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CRYSTALS OF THE *ESCHERICHIA COLI* MEMBRANE-ASSOCIATED GLYCOSYLTRANSFERASE (MurG) PROTEIN, ATOMIC COORDINATES AND THREE DIMENSIONAL STRUCTURES THEREOF, ATOMIC COORDINATES AND THREE DIMENSIONAL STRUCTURES OF BINDING DOMAINS THEREOF, IMAGES THEREOF, AND METHODS OF CRYSTALLIZING MurG PROTEINS, MODELS OF UDP GLYCOSYLTRANSFERASES, MurG PROTEINS AND BINDING SITES, METHODS OF MAKING MODELS, METHODS OF USING MODELS OF MURG, COMPOUNDS THAT BIND, INHIBIT OR STIMULATE MURG PROTEINS, AND THERAPEUTIC COMPOSITIONS THEREOF

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FIELD OF THE INVENTION

The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone of the MurG protein and images thereof. The present invention further relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains; and images thereof. The present invention also relates to computer readable media encoded with sets of the three dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and the conserved amino acid residue sidechains of the MurG protein, the donor nucleotide binding site, the acceptor binding site, and the membrane association site. The present invention relates to methods of crystallizing MurG proteins.

The present invention relates to models of three dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three dimensional structure of

The elucidation of the protein structure of a MurG protein is of importance in the identification and formulation of anti-bacterial agents. Until the discovery of the present invention, the structure and resulting mechanism by which MurG functions was not known. Thus, despite the important role of MurG in peptidoglycan synthesis, development of useful agents for treatment or diagnosis of disease was hindered by lack of structural information of the protein.

In order to obtain structural information on a MurG Protein, it is important to have purified, active enzyme. The demonstration of activity requires a suitable assay, which in turn requires access to the natural substrates or analogues thereof. The study of MurG was hampered by difficulties obtaining and handling the lipid-linked NAM substrate (commonly known as Lipid 1). This problem was overcome by Walker and coworkers, who developed a synthetic route to a set of substrate analogues of Lipid I that were shown to function as glycosyl acceptors in a glycosyl transfer reaction catalyzed by MurG. Some of these substrate analogues are freely water soluble, making it possible to monitor the activity of purified *E. coli* MurG in buffer in the absence of natural or artificial membranes or detergents.

The linear nucleic acid and amino acid sequences of *E. coli* MurG were reported in 1992. Subsequently, the nucleic acid and amino acid sequence of *B. subtilus* MurG was reported. Since then, many bacterial genomes have been sequenced and the information has been deposited in databases. Information based only on linear sequences, however, cannot accurately predict the three-dimensional structure of the protein and its functional domains.

Therefore, there is a need in the art to elucidate the three-dimensional structure of a MurG protein. One three dimensional structure of a MurG protein can be used to construct models of other MurG proteins and to facilitate the structure determination of crystalline forms of other MurG proteins. Structures and models of MurG proteins can also be used to design proteins containing only the donor binding site or the acceptor binding site. These proteins can be used in assays, including NMR-based assays, to identify -- or characterize the mode of binding of -- ligands that bind in or near the vicinity of the substrates. These ligands or compounds can then be used as leads for the design of inhibitors that have therapeutic activity. Structures and models of MurG proteins can also be used in computer-based drug design.

SUMMARY OF THE INVENTION

The present invention relates to crystalline *Escherichia coli* MurG protein. Obtaining such crystals is an unexpected result. It is well known in the protein crystallographic art that obtaining

crystals of quality sufficient for determining the structure of a protein is unpredictable. In particular, obtaining crystals of quality sufficient for determining the three-dimensional (3-D) structure of MurG has not been achievable until the crystallization of MurG as disclosed in the present application. As such, determination of the three-dimensional structure of MurG has not been possible until the discovery of the present invention. Additionally, until the discovery of the present invention, derivation of the three-dimensional structure and models of other MurG proteins has not been possible. The present inventors are also the first to define the three-dimensional structure and provide three-dimensional models for drug design for MurG proteins.

Accordingly, one object of the present invention is to provide crystals of sufficient quality to obtain a determination of the three-dimensional atomic coordinates and structures of MurG to high resolution, preferably to the resolution of less than 2.0 angstroms (Å). The present invention also provides methods for producing crystalline MurG protein.

The value of the crystals of *E. coli* MurG protein extends beyond merely being able to obtain such crystals. The knowledge obtained concerning the MurG crystal structure, for example, has been used by the present inventors to define the heretofore unknown tertiary structure of the MurG protein and to identify the location of the glycosyl donor and glycosyl acceptor binding domains, as well as the location of the amino acid residues that are invariant in all MurG proteins. This information can be used to design inhibitors of MurG that have therapeutic utility. The atomic coordinates of *E. coli* MurG also are used to model the heretofore unknown tertiary structures of other MurG proteins having substantially related linear amino acid sequences, such as for MurG proteins from other microorganisms. It is anticipated that homology models can be constructed even from amino acid sequences with relatively low homology because the present inventors have identified the location of the invariant amino acid residues in MurG. The relative spatial orientations of such residues is expected to be conserved in all MurG proteins.

Comparison of nucleic acid and amino acid sequences of MurG proteins indicates that the linear amino acid sequences can vary significantly. Homology between MurG proteins from different microorganisms varies from less than 30% to greater than 90%, reflecting the evolutionary relationship between the organisms. The low homology between distantly related MurG homologues is not believed to reflect significantly different folded structures. It is well known that many amino acid sequences are capable of adopting the same general fold. *E. coli* MurG contains an alpha/beta folding pattern, one of the most common folds known in proteins. It

is likely that all MurG homologues contain a similar alpha/beta fold despite the differences in the linear amino acid sequences. What gives these proteins their identity is not the general fold, but the specific details - i.e., the presentation of certain amino acids on the folded structure. The present inventors have identified the location in *E. coli* MurG of a set of residues that are invariant in all MurG homologues. It is to be expected that these residues would adopt a similar spatial location with respect to the folded structure in all MurG homologues. Therefore, these invariant residues, which have been selected by evolution as the critical residues for the binding and catalytic function of the protein, provide essential information on the location of the active site and on critical contacts to the substrates/products. They also serve as constraints that make it possible to, predict the three-dimensional structures even of distantly related MurG homologues. Thus, knowledge of the three-dimensional structure of the *E. coli* MurG protein has provided a starting point for investigation into the structure of all MurG proteins.

Accordingly, a object of the present invention is to provide information regarding the atomic coordinates and three-dimensional structures of (1) the MurG protein, (2) the α-carbon backbone of the MurG protein, (3) the α-carbon backbone and conserved amino acid residues of the MurG protein, (4) the donor nucleotide binding site, (5) the acceptor binding site, and (6) the membrane association site MurG proteins.

It is also an object of this invention to solve the three-dimensional structure of UDP-glycosyltransferases, in particular target MURG proteins, and to determine their structure and/or atomic coordinates. Further, it is an object of this invention to use the structure or atomic coordinates of the *E. coli* MurG crystal to solve the structure of different MURG protein crystals, or a crystal of a mutant protein, homolog or co-complex of MurG.

The present invention relates to models of three dimensional structures of UDP-glycosyltransferases, in particular MurG proteins, based on the atomic coordinates of crystalline *E. coli* MurG protein.

It is a further object of this invention to provide UDP-glycosyltransferase enzyme mutants characterized by one or more different properties as compared with wild-type MURG. These properties include altered surface charge, increased stability to subunit dissociation, altered substrate specificity or higher specific activity. MURG mutants are useful to identify those amino acids that are most important for the enzymatic activity of MURG. This information, in turn, allows the design of improved inhibitors of MURG as compared with peptidic MURG inhibitors.

Another object of the present invention is to provide computer readable mediums encoded with a set of three-dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

Another embodiment of the present invention provides three-dimensional and two-dimensional computer images of the three dimensional structure of MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

The knowledge of the three dimensional structure of MurG also provides a means for designing proteins that have altered beneficial functions by analyzing the structure and interactions between individual amino acids of the protein. For example, the present inventors have shown that E. coli MurG consists of two domains separated by a cleft. Noncovalent interactions between the two domains are not extensive. The present inventors have shown that the domains fold independently and can, therefore, be expressed independently either alone or as part of a recombinant protein containing the acceptor binding site from one MurG homologue and the donor binding site from another MurG homologue. It would be expected that the domains of other MurG proteins could also be expressed independently, either alone or as chimaeras with other MurG domains. Independently expressed domains of the protein are useful for discovering ligands that bind to the individual domains.

The knowledge of the three-dimensional structure of *E. coli* MurG protein and models of other MurG proteins also provides a means for designing and producing compounds that regulate, inhibit or antagonize functions of the MurG protein (i.e., structure based drug design). For example, chemical compounds can be designed to block binding of UDP-GlcNAc to a MurG protein using various computer programs and models.

It is also an object of this invention to use the structure coordinates and atomic details of MURG, or its mutants or homologues or co-complexes, to design, evaluate computationally, synthesize and use inhibitors of MURG that avoid the undesirable physical and pharmacologic properties of peptidic MURG inhibitors. Another embodiment of the present invention is a composition comprising MurG protein in a crystalline form.

Yet another embodiment of the present invention is a method for producing crystals of MurG, comprising combining MurG protein in a suitable buffer with a suitable amount of a reservoir buffer containing a detergent, and inducing crystal formation to produce said MurG crystals.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1. Pathway for peptidoglycan biosynthesis.

FIG. 2. Overall architecture of MurG. A. Stereo view of the MurG structure. The N domain is shown in purple; the C domain is shown in green. The figure was generated with the programs MOLSCRIPT (Klaulis, 1991) and RASTER3D) (Merrit & Murphy, 1994). B. Topology diagram of MurG.

FIG. 3. Identification of critical residues in MurG and related glycosyltransferases. **A**. Sequence alignment of *E. coli* MurG with homologs from seven other bacterial strains, deliberately chosen to represent a disparate group of organisms. The secondary structure of *E. coli* MurG is shown above the sequences. Gaps mapping to the loop regions of E. coli MurG suggest that some sequences include other structural elements. Residues highlighted in blue are invariant among the eighteen MurG sequences available. Residues highlighted in yellow are identical in 85% of the eighteen homologs, while in the remaining 15%, only closely related amino acid substitutions are found. Highly conserved residues that do not meet the stringent criteria established for highlighting are shown in the consensus sequence. A consensus motif for UDP-glucuronosyltransferases is also shown. Numbering is with respect to the overexpressed *E. coli* MurG construct, which contains an additional N-terminal methionine. **B**. Mapping of the G loops and other highlighted residues from Fig. 3a in red on the MurG structure. Side chains for highly conserved residues are also shown. **C**. Model for the proposed UDP-binding subdomain found in many UDP-glycosyltransferases based on the *E. coli* MurG structure. Conserved residues in UDP-glucuronosyltransferases are highlighted in red. Side chains are shown for residues that are located near the cleft and may be involved in substrate binding. The glutamate residue is proposed to interact with the ribose sugar. The dotted loop varies in length within the MurG family and in other UDP-sugar transferases, but the N and Q on the following helix are invariant. Note that the UDP-glucuronosyltransferases contain a conserved D preceding the Q, which is not shown on this model.

The term "mutant" refers to a MurG polypeptide, i.e., a polypeptide displaying the biological activity of a wild-type MurG, characterized by the replacement of at least one amino acid from the wild-type, *E. coli* MURG sequence according to Ikeda, et al., Nucleic Acids Res. 1990, and Mengin-LeCreuix et al., Nucleic Acids Res. 1990. Such a mutant may be prepared, for example, by expression of MURG cDNA previously altered in its coding sequence by PCR-based mutagenesis method.

MurG mutants may also be generated by site-specific incorporation of unnatural amino acids into MURG proteins using the general biosynthetic method of Noren, C. J., et al., Science, 244, pp. 182-188 (1989). In this method, the codon encoding the amino acid of interest in wild-type MURG is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis (described in detail, infra). A suppressor tRNA directed against this codon is then chemically aminoacylated in vitro with the desired unnatural amino acid. The aminoacylated tRNA is then added to an in vitro translation system to yield a mutant MURG enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant MURG by expression of MURG-encoding cDNAs in auxotrophic E. coli strains. Hendrickson, W. A. et al., EMBO J., 9(5), pp. 1665-1672 (1990). In this method, the wild-type or mutagenized MURG CDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "altered surface charge" means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to wild-type MURG. This is preferably achieved by mutation of at least one amino acid of wild-type MURG to an amino acid comprising a side chain with a different charge at physiological pH than the original wild-type side chain.

The change in surface charge is determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the isoelectric point of the wild-type MURG molecule.

The term "altered substrate specificity" refers to a change in the ability of a mutant MURG to cleave a substrate as compared to wild-type MURG.

The "kinetic form" of MURG refers to the condition of the enzyme in its free or unbound form or bound to a chemical entity at either its active site or accessory binding site.

A "competitive" inhibitor is one that inhibits MURG activity by binding to the same kinetic form, of MURG, as its substrate binds-thus directly competing with the substrate for the active site of MURG. Competitive inhibition can be reversed completely by increasing the substrate concentration.

An "uncompetitive" inhibitor is one that inhibits MURG by binding to a different kinetic form of the enzyme than does the substrate. Such inhibitors bind to MURG already bound with the substrate and not to the free enzyme. Uncompetitive inhibition cannot be reversed completely by increasing the substrate concentration.

A "non-competitive" inhibitor is one that can bind to either the free or substrate bound form of MURG.

Those of skill in the art may identify inhibitors as competitive, uncompetitive or non-competitive, by computer fitting enzyme kinetic data using standard equations according to Segel, I. H., Enzvme Kinetics, J. Wiley & Sons, (1975). It should also be understood that uncompetitive or non-competitive inhibitors according to this invention may bind to the accessory binding site.

The term "homolog" means a protein having at least 25% amino acid sequence identity with MURG or any functional part of MURG, and including certain invariant amino acid residues corresponding to G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E.coli* MurG sequence set forth in Figure 3a) and also including three glycine rich loops. A homolog may contain- some or all of the invariant residues.

The term "co-complex" means MURG or a mutant or homologue of MURG in covalent or non-covalent association with a chemical entity or compound.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a MurG molecule or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be dovalent.

The term ".beta.-sheet" refers to the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run “parallel” all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

The terms "atomic coordinates" or "structure coordinates" refer to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a MurG molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

The term "heavy atom derivatization" refers to the method of producing a chemically modified form of a crystal of MURG. In practice, a MurG crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal, uranyl acetate or mercuric chloride, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the enzyme. Blundel, T. L. and N. L. Johnson, Protein Crystallography, Academic Press (1976).

Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for MURG or MURG homologues or MURG mutants that have a root mean square deviation of protein backbone atoms (N, C.alpha., C and O) of less than 0.75 Å when superimposed--using backbone atoms--on the structure coordinates listed in Table 1, Table 2 or Table 3 shall be considered identical.

The term "unit cell" refers to a basic parallelepiped shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary model of a MurG crystal whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (e.g., MURG coordinates from Table 1, 2, or 3) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. Lattman, E, "Use of the

Rotation and Translation Functions", in Methods in Enzymology, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972). Using the structure coordinates of MURG provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of MURG or of a different crystal form of MURG.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the discovery of the three-dimensional structure of the crystalline form of the *E. coli* MurG protein, models of such three-dimensional structures, a method of structure based drug design using such structures, methods to identify ligands or compounds that interact or bind with such structures, the compounds identified by such methods, and the use of such compounds in therapeutic compositions.

More particularly, the present invention relates to novel crystals of *E. coli* MurG protein, methods of production of such crystals, three dimensional coordinates of MurG protein, MurG structures and models derived from the *E. coli* MurG structure, and uses of such structures and models to derive other MurG structures and in ligand discovery and drug design strategies.

The present invention also relates to three-dimensional structures and coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, structures and models of the binding sites, and uses of such structures and models to derive the binding sites of other MurG proteins and in drug design strategies.

Solely for ease of explanation, the description of the invention is divided into the following sections: (1) crystals of MurG protein; (2) methods of crystallization; (3) threedimensional crystal coordinates and structure of E. coli MurG; (4) three-dimensional coordinates and structure of the donor nucleotide binding site of MurG; (5) coordinates and structure of the acceptor binding site of MurG; (5) three dimensional coordinates and structure of the membrane association site; (6) two dimensional and three dimensional images of the protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; and (7) computer readable mediums comprising the three dimensional coordinates of the MurG protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; (8) images of structures of MurG protiensand binding sites; (9) models of MurG proteins and binding sites thereof and methods of using the structure of MurG to determine the structures of other MurG proteins and binding sites;

(10) structure based drug design using models of MurG protein and binding site structures; (11) compounds derived from structure based drug design; and (12) therapeutic compositions using drugs designed from structure based drug design.

CRYSTALS

One embodiment of the present invention includes a pomposition comprising a MurG protein in a crystalline form (i.e., MurG crystals). As used herein, the terms (crystalline MurG" and "MurG crystal" both refer to crystallized MurG protein and are intended to be used interchangeably. More particularly, an embodiment of the present invention includes a composition comprising an *E. coli* MurG protein in a crystalline form. Preferably, a crystalline MurG is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 1. A MurG crystal of the present invention comprises any crystal structure and preferably precipitates as a triclinic crystal. Preferably, a composition of the present invention includes MurG crystal molecules arranged in a crystalline manner in a P1 space group with two molecules per assymmetric unit so as to form a unit cell of dimensions a=60.613 Å, b=66.356 Å, c=67.902 Å, α=64.294, β=83.520, γ=65.448. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates to a resolution of about 3.0 Å, preferably to about 2.4 Å, and more preferably to about 1.8 Å.

Another embodiment of the present invention includes crystalline MurG protein co-crystallized with a donor nucleotide or substrate or substrate analog. Preferably, a donor nucleotide is UDP or UDP-GlcNAc (UDP-N-acetylglucosamine) or an analog thereof. The substrate or substrate analog is preferably Lipid I or Lipid II, or analogs of Lipid I or Lipid II. More specifically, Lipid I and II analogs are as described in PCT/US99/02187, published as W099/38958 and US Provisional Application Nos.60/122,966 filed March 3, 1999 and 60/137,696 filed June 4, 1999, and International Application No. PCT/USOO/05554 entitled "Bacterial transglycosylases: Assays for monitoring the activity using lipid II substrate analogs and methods for discovering antibiotics," all incorporated herein by reference in their entirety.

Included in the present invention, a variety of MurG proteins from numerous organisms can be used to prepare MurG crystals, including but not limited to, microorganisms such as bacteria, higher-order bacteria, then-nal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not

limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

In another embodiment of the present invention, the MurG proteins or fragments thereof, mutants or homologs are expressed in, for example, an *E. coli* host cell for use expressing sufficient quantities of sufficiently purified protein to form crystals. The present inventors have demonstrated that it is possible to express *Enterococcus faecalis* MurG in *E. coli* cells - so the MurG proteins from many organisms can be cloned into expression vectors suitable for expression in *E. coli* cells. This would facilitate obtaining sufficient quanitites of isolated or purified MurG proteins.. The expression of E. *faecalis* MurG protein in *E.* coli host cells is performed, for example, by expressing the E. *faecalis* MurG gene cloned into a pET21b expression vector and transformed into an *E. coli* host cell. The MurG protein is over-expressed with a C-terminal his tag (LEHHHHHH) which allows the protein to be purified using a His-tag affinity column. The protein is then crystallized and the atomic coordinates are determined using X-ray diffraction and methods known to those skilled in the art.

It is another embodiment of the present invention to provide for the construction and expression of chimeric MurG proteins to enable the crystallization and determination of the three dimensional coordinates of such chimeras. For example, if there are problems obtaining or crystallizing MurGs from other organisms, the present invention provides information that makes it possible to make chimaeric proteins containing the donor or acceptor binding site from *E. coli* MurG and the corresponding acceptor or donor binding site from another organism. Chimaeric proteins could be easier to express, handle, or crystallize. For example, we have found that *E. faecalis* MurG is more difficult to solubilize that *E. coli* MurG (requiring more detergent). It is believed that the problems are related to the acceptor binding domain having a stronger affinity for the bacterial membranes. To overcome this problem, one can attach the donor binding domain of *E. faecalis* to the *E. coli* acceptor binding site and determine structure to see details of *E. faecalis* donor binding domain.

According to the present invention, crystalline MurG can be used to determine the ability of a chemical compound to bind to a MurG protein in a manner predicted by a structure based

drug design method of the present invention. Preferably, a MurG crystal is soaked in a solution containing a chemical compound of the present invention. Binding of the chemical compound to the crystal is then determined by methods standard in the art. Thereby, the co-crystal of MurG and a compound of interest is determined.

METHODS OF CRYSTALLIZATION

The present invention includes a method for producing crystals of MurG proteins, comprising: combining MurG protein with a reservoir solution and inducing crystal formation to produce MurG crystals. Another embodiment of the present invention, a method for producing crystals of MurG protein comprises combining MurG protein with UDP-GlcNAc in a 1:3 ratio and with a reservoir solution and inducing crystal formation to produce MurG crystals.

Preferably, crystals of MurG are formed using a solution containing a range of MurG protein from about 1 mg/ml to about 20 mg/ml, more preferably above 5 mg/ml, limited only by the solubility of the protein, which may vary depending on the specific amino acid sequence. A reservoir solution contains the buffer, the precipitant, and additives if necessary. A suitable reservoir buffer of the present invention comprises NaMES (2-[Nmorpholinolethanesulfonic acid, sodium salt) buffer, NaHEPES (N-[2hydroxyethyl]piperazine-N'-[2-ethanesulfonic acid, sodium salt) buffer, Tris (tris[hydroxymethyl]aminomethane) buffer, and any buffer which has the PKa between 5.5 and 8.0. A suitable NaMES buffer solution has a pH range from about 5.6-6.5. Most preferably, the NaMES buffer has a pH of about 6.5. The precipitant comprises ammonium sulfate, saturated sodium and potassium tartrate and polyethylene glycol. A suitable concentration of ammonium sulfate can range from 0.8 M to 1.5 M. Most preferably, the ammonium sulfate concentration is about 0.96 M. A suitable additive comprises detergents like Triton X-100 and n-octyl-beta-glucoside. The concentration of Triton X-100 can range from 0.1% to 1%. Most preferably, the concentration of Triton X-100 is 0.4%.

In a preferred embodiment, MurG crystals are produced by a method comprising concentrating MurG protein in a buffer solution, mixing the protein concentrate with UDP-GlcNAc in a 1:3 molar ratio, mixing equal volumes of protein solution with a reservoir solution, and inducing crystal formation to produce MurG crystals.

In a particular embodiment of the invention, MurG crystals are produced by a method comprising concentrating MurG protein to 10 mg/ml in a buffer of 20 mM TrisHCl, pH 7.9/150mM NaCl and 50 mM EDTA; mixing the protein concentrate with UDP-GlcNAc in a

1:3 molar ratio; mixing equal volumes of protein solution with a reservoir solution comprising (0. 1 M NaMES, pH 6.5, 0.96 M $(NH_4)_2SO_4$, 0.4% TRITON® X-100, and 10 mM dithiolthreitol (DTT)), and inducing crystal formation using hanging drop vapor-diffusion. This preferred method is described in greater detail in Example 1.

Supersaturated solutions of MurG protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of MurG protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, a MurG protein solution is combined with a reservoir solution of the present invention that will cause the MurG protein solution to become supersaturated and form MurG crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the ranue of from about 15°C to about 30°C, more preferably from about 20°C to about 25°C, and most preferably at a constant temperature of about 22° C.

In another preferred embodiment, the present invention includes a method to produce crystals of MurG protein comprising the steps of: (a) preparing an about 10 mg/ml solution of MurG protein in a Tris-HCl buffer, (b) mixing UDP-GlcNAc with the Mur-G protein solution in a 3:1 molar ratio, (c) dropping 2 μl droplet of this protein sample onto a coverslip, (d) adding an equal volume of reservoir solution to this droplet and inverting this over a well containing about 1 ml of the reservoir solution; and (e) incubating until crystals of MurG form.

Any isolated MurG protein can be used with the present method. An isolated MurG protein can be isolated from its natural milieu or produced using recombinant DNA technology (e.g., polymerase chain reaction (PCR) amplification, cloning) or chemical synthesis. To produce recombinant MurG protein, a nucleic acid molecule encoding a MurG protein can be inserted into any vector capable of expressing the nucleic acid in a host cell. Suitable and preferred nucleic acid molecules to include in recombinant vectors of the present invention are as disclosed herein. Such suitable and preferred nucleic acid molecules include numerous MurG encoding genes that have been isolated to date, and that will be isolated in the future. A preferred nucleic acid molecule of the present invention encodes a homologue of MurG. Homologues of MurG can be recognized by the presence of certain conserved amino acid residues or sequences.

A sequence alignment for six MurG sequences is shown in fig. 3A. Highlighted residues include those that are invariant or almost invariant across all MurG proteins. A nucleic acid molecule

of the present invention can encode any portion of a MurG protein, preferably a full-length MurG protein or either of the two domains. A more preferred nucleic acid molecule to include in a recombinant vector, and particularly in a recombinant molecule, includes a nucleic acid molecule encoding a protein having the amino acid sequence represented by amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, 084766, 069552,)67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. Further, examples of nucleic acid molecules encoding MurG proteins have been deposited in NCBI, Genbank, and have Accession Nos. AL162758, AE00228 1, D90917, AF110367, AL139077, AJ242646, AE000520, AE000511, L42023, U00096, NC-000922, AE000783, AE000657, AE001348, AF099188, AR048673, AR048672, AF179611, AL022602, AL109663, X55034, AE000621, D10602, AE001670, X64259, Y13922, U10879, AE001535, AF068902, AJ235271, AE000118, AE001227, AE001176, U94707, Z95388, U32793, AE000727, D84504, Z99111, D10483, X52644, X52540, and L24773. These sequences are known and are publicly available. Further, as additional genomes and genes are sequenced, more MurG encoding nucleotide sequences will become available, and can be used in the present invention.

In specific embodiments of the invention, the protein sequence of *E. coli* MurG was reported in 1990 (Ikeda et al. Nucleic Acids Res. 1990, 19:4014; and Mengin Lecreuix, D. et al., Nucleic Acids Res. 1990, 18:2810.). *E. coli* genomic DNA can be purified from *E. coli* or purchased from ATCC, or the gene for *E. coli* MurG is cloned into a plasmid can be obtained from numerous sources. Primers were designed to the portions of the gene corresponding to the N and C termini of the protein. The primers also encoded restriction enzyme sites outside the protein coding region. The gene sequence was amplified; the corresponding double stranded nucleic acid molecule was cut with appropriate restriction enzymes for cloning into a commercially available expression vector (pET expression vectors available from Novagen provide for numerous

variations of MurG protein - wild-type or fusion proteins or proteins with affinity tags at N or C terminus. We have worked with several constructs but found that MurG with a His-tag at C-terminus crystallized best; the protein sequence contained an extra methionine at N-terminus and eight extra residues at C terminus, six of which were histidines. The vector used was pET21b. (as described in Ha et al. J. Am. Chem. Soc. 121, (1999) 8415-8426 hereby incorporated by reference in its entirety).

A recombinant vector of the present invention can be either RNA (probably not) or DNA, and typically includes, but is not limited to, a virus or plasmid. Any recombinant vector and host cell that provides for expression of a MurG protein encoding mucleic acid sequence can be used in the present invention to express MurG protein for crystallization. Preferred vectors are engineered for high level expression in *E. coli* such as, but not limited to, pET vectors. We have found that over-expression of Murg from either *E. coli* or *E. faecalis* in *E. coli* cells is not toxic and, thus, this approach will work for other MurG proteins.

As used herein, an expression vector is a DNA vector that is capable of transforining a host cell and of affecting expression of a specified nucleic acid molecule. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including bacterial, fungal, and other microorganisms cells. Preferred expression vectors of the present invention direct expression in bacterial cells from a plasmid. A preferred recombinant molecule of the present invention comprises pET21b with *E. coli* MurG gene cloned into the Nde I and Xho I sites.

An expression vector of the present invention can be transformed into any suitable host cell to form a recombinant cell. A suitable host cell includes any cell capable of expressing a nucleic acid molecule inserted into the expression vector. For example, a procaryotic expression vector can be transformed into a bacterial host cell. If the expression vector contains a T7 promoter then a source of T7 RNA polymerase must be provided to induce expression. Some host cells contain the T7 RNA polymerase gene in a repressed state. Expression of T7 RNA polymerase can be induced with a chemical signal such as IPTG or heat. Alternatively, a source of T7 RNA polymerase can be introduced at the appropriate time by infection with a phage containing a copy of T7 RNA polymerase. A wide range of hosts strains can be infected with a suitable phage. Some host strains have been engineered to contain inducible copies of T7 RNA polymerase gene. Such host strains include BL21(DE3) and derivatives thereof. A preferred host strain of the present invention is BL21(DE3)pLysS or BL21(DE3)pLysE, which are commercially available from

Novagen and can be readily transformed with a DNA plasmid vector containing a MurG gene under the control of the T7 promoter. As already stated above, a preferred vector is a pET vector, preferably containing a restriction enzyme site pennitting cloning of the gene as a fusion containing a C-terminal his tag.

In a preferred embodiment, one method to isolate MurG protein useful for producing MurG crystals includes recovery of MurG protein having a C-terminal LEHHHHHH (His tag) sequence purified as described in Ha et al. (1999, J. Amer. Chem. Soc. 121:8415-8426). One of skill in the art is able to modify this procedure in order to purify other proteins can be produced as C-terminal histadine (his) tags. The purification conditions for specific MurG proteins will vary depending upon the particular characteristics of the proteins such as their isoelectric point, molecular weight, etc. It is known that the isoelectric points of different Murg homologues vary a bit, although they are generally relatively high. Also, some Murg homologues may be more hydrophobic than others, which will mean differences in amount of detergent necessary for purification. It is likely that all the Murg homologues can be purified over nickel affinity columns using the C-terminal his-tag as a handle. Those skilled in the art of protein purification will know how to modify purification parameters depending upon the protein characteristics, in order to purify the protein for crystallization.

STRUCTURE OF MURG PROTEIN

One embodiment of the present invention includes a model of a MurG protein, in which the model represents a three dimensional structure of a MurG protein. Another embodiment of the present invention includes the three dimensional structure of a MurG protein. A three dimensional structure of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 1. According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 1) to allow the three dimensional structure of another MurG protein to be modeled or calculated using the particular set of atomic coordinates defining the three dimensional configuration of the MurG protein. For example, but not meant to be a limitation, homology modeling can be done using the linear sequence of a different MurG and E. coli coordinates; molecular replacement can allow the solution of a different MurG structure using the E. coli MurG coordinates and experimental data

such as x-ray diffraction pattern from a different MurG crystal. According to the present invention, a three dimensional structure of a given portion or chain of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the α-carbon or C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the common amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å.

In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the common amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the common amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the common amino acid side chains have the recited average RMSD value.

In more preferred embodiments of the present invention, a large number of different "rotamers" or "rotational isomers" of the MurG protein are encompassed by three dimensional

structures of the invention in which the amino acid side chains are at a variety of positions in crystalline forms of the protein or for the protein in solution. Different rotamers refer to molecules of identical configuration may be distinguished as having different conformations after rotation about the various molecular bonds. Therefore, while the same or similar amino acids may be present, the exact location will vary depending upon the freedom of rotation of the bonds due to hydrogen bonding, and other molecular forces.

STRUCTURE OF THE α-CARBON BACKBONE OF MURG AND THE α-CARBON BACKBONE AND CONSERVED AMINO ACID RESIDUES

The present invention includes the three dimensional structure of the α-carbon or C-alpha backbone of a MurG protein, in particular the *E. coli* MurG protein. A three dimensional structure of the C-alpha backbone of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 2.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value. The C-alpha backbone of MurG proteins is expected to be more conserved than the location of the particular amino acid residue side chains.

The present invention also includes the three dimensional structure of the (α-carbon or C-alpha backbone and conserved or invariant amino acid residue side chains of a MurG protein, in particular the *E. coli* MurG protein. A three dimensional structure of the C-alpha backbone and conserved amino acid residues of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 3. The conserved amino

acids are highlighted in blue in Figure 3a and include G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a).

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å, for the C-alpha backbone and conserved amino acid residue atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average rootmean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

STRUCTURE OF THE DONOR NUCLEOTIDE BINDING SITE OF MURG PROTEINS

An embodiment of the present invention includes the three dimensional structure of a donor nucleotide binding site of a MurG protein, in particular an E. coli MurG protein. A more preferred embodiment of the present invention includes a three dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three dimensional structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4. In a preferred embodiment, the donor nucleotide binding site is a UDP-GlcNAc binding site of a MurG protein.

As described in Example 1, the donor nucleotide binding site is located in the C-terminal domain (see Fig. 4a). This binding site is based on the comparison of ß-glucosyltransferase (BGT) and *E. coli* MurG and based on experiments done in our laboratory showing that the isolated C domain binds to a UDP-hexose column (See Example 1). The atomic coordinates of Table 4 set forth the donor nucleotide binding site three dimensional structure without a donor nucleotide such as UDP-GlcNAc bound to the MurG protein.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a donor nucleotide binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 4) to allow the three dimensional structure of the donor nucleotide binding domain to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three dimensional configuration of the donor nucleotide binding site of a MurG protein. According to the present invention, a three dimensional structure of a given donor nucleotide binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG. Since the atomic coordinates of Table 4 were obtained from the *E. coli* MurG crystal protein without a donor nucleotide bound, there will be some variation from the atomic coordinates of the donor nucleotide binding site when a nucleotide is bound vs. unbound. Therefore, a structure "substantially conforming" to that represented by the atomic coordinates in Table 4, will include a structure obtained from co-crytallization of the protein with a donor nucleotide.

More particularly, a structure that substantially conforms to a given s6t of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and more preferably less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved or invariant amino acid side chains located within the binding site. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins within the donor nucleotide binding site. The conserved amino acid residues of the donor nucleotide binding site have been identified as I125, R261, G263, A264, E269, P281, Q289, N292 and, A293 (as numbered in the *E.*

coli MurG sequence set forth in Figure 3a) and the G loop found between residues numbered 190-195 having residues G190, G191, S192, G194, and A195. Some or all of these conserved residues are necessary for binding the nucleotide donor.

Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF THE ACCEPTOR BINDING SITE OF MURG PROTEIN

An embodiment of the present invention includes the three dimensional structure of an acceptor binding site of a MurG protein. A three dimensional structure of a acceptor binding site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 5. A more preferred embodiment of the present invention includes a three dimensional structure of an acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates Table 5.

According to the present invention, the use of the term "acceptors" refers to Lipid I and analogues thereof. For the purposes of obtaining co-crystals containing acceptor analogues bound to the acceptor binding site better, the analogues need not be functional acceptors in a MurG assay. In particular embodiments of the present invention, the acceptor is selected from the group consisting of, but not limited to Lipid I, and analogs of Lipid I (see compounds described in Ha et al., J. Amer. Chem. Soc. 1999, vol. 121:8415-26, incorporated by herein by reference in its entirety).

As described in Example 1, the acceptor binding site is located in the N-terminal domain of a MurG protein (see Fig. 3a and 4c). The acceptor binding site or domain is characterized by three highly conserved regions, two of which are glycine-rich loops (also referred to as "G loops") that face the cleft between the C-terminal and N-terminal domains. The conserved residues of the

acceptor binding site comprise G14, G15, G18, H19, G104, H124, and E125 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and two conserved G loop structures.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of an acceptor binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 5) to allow the three dimensional structure of the acceptor binding site to be modeled or calculated (i.e., by homology modeling) using the particular set of atomic coordinates defining the three dimensional configuration of the acceptor binding site of a MurG protein. According to the present invention, a three dimensional structure of a given acceptor binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to the conserved or invariant amino acid side chains that are common to MurG proteins. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF A MEMBRANE ASSOCIATION SITE OF MurG PROTEIN

An embodiment of the present invention includes the three dimensional structure of a membrane association site of a MurG protein, A three dimensional structure of a membrane association site of a MurG protein encompassed by the present invention substantially conforms

with the atomic coordinates represented in Table 6. A more preferred embodiment of the present invention includes a three dimensional structure of an acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates in Table 6.

According to the present invention, the use of the term "membrane association site" refers to the region of a MurG protein that associates with cytoplasmic surface of bacterial membranes where it performs the reaction of coupling a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG protein structure shows a hydrophobic patch consisting of residues I75, L79, F82, W85, and W116 in the N-domain. The membrane association site is where the MurG protein associates with the bacterial membranes, and that it is target for inhibitors if we find that a) we can bind to it with another molecule; b) we can disrupt membrane association by binding to it; or c) disrupting membrane association inhibits activity.

As described in Example 1, the membrane association site is located in the N-terminal domain of a MurG protein (see Fig. 4c). The location of the membrane association site is in close proximity to the acceptor binding site and membrane association in this patch would bring the two M-terminal G-loops close to the membrane surface where the diphosphate portion of the acceptor is located.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a membrane association site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 6) to allow the three dimensional structure of the membrane association site to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three dimensional configuration of the membrane association site of a MurG protein. According to the present invention, a three dimensional structure of a given membrane association site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the structural elements in the site, and more preferably, less than about 1.3 Åfor the structure elements in each site, and, in increasing

preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and more preferably, less than about 0.3 Å for the structural elements in each site. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of α-carbon backbone and conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved α-carbon backbone and conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the α-carbon backbone and conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the α-carbon backbone and conserved acid side chains have the recited average RMSD value, and most preferably, about 100% of the α-carbon and conserved amino acid side chains have the recited average RMSD value.

COMPUTER READABLE MEDIUM

Another embodiment of the present invention relates to a computer-readable medium encoded with, a set three dimensional coordinates seleceted from the group consisting of the three dimensional coordinates represented in Table 1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, the three dimensional coordinates represented in Table 5, or the three dimensional coordinates represented in Table 6, wherein using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

Preferably, the three dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Yet another embodiment of the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 1, wherein using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. In other embodiments, the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 2, Table 3, Table 4, Table 5 or Table 6, wherein using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

IMAGES

One embodiment of the present invention relates to a two dimensional image of an *E. coli* MurG protein including those illustrated in Figures 3-4. Most of these figures were drawn with the MOLSCRIPT program. Preferably, the two dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Another embodiment of the present invention includes a three dimensional computer image of the three dimensional structure of a MurG protein, preferably the *E. coli* MurG protein. Suitable structures of which to produce three dimensional computer images are disclosed herein.

Preferably, a computer image is created to a structure substantially conforming with the three dimensional coordinates represented in Table 1.

Another embodiment of the present invention includes an image of an MurG protein that is generated when a set of three dimensional coordinates comprising the three dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file as a three dimensional image. Suitable structures to image are disclosed herein. Preferably, the three dimensional structures are of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG. Most preferably, the MurG protein is the E. coli MurG protein described herein. A computer image of the present invention can be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Helenebrgsgatan 21 C, SE- 11713, Stockholm, Sweden), the graphical display program O (Jones et al., Acta Crystallography, vol. A47, p. 110, 1991), or the graphical display program GRASP. Suitable computer hardware useful for producing an image of the present invention are known to those of skill in the art. Preferred computer hardware includes a Silicon Graphics Workstation.

MODELS OF MURG PROTEINS AND BINDING SITES

According to the present invention, a three dimensional structure of the *E. coli* MurG protein and its binding sites of the present invention can be used to derive a model of the three dimensional structure of another MurG protein and its binding sites (i.e., a structure to be modeled). As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute a protein or binding site. Also, as used herein, the term "model" refers to a representation of a tangible medium of the three dimensional structure of a protein, polypeptide or peptide, or binding site of a protein. For example, a model can be a representation of the three dimensional structure in a electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available

from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosyrn Technologies, San Diego, CA. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Computer screen images and pictures of the model can be visualized in a number of formats including space-filling representations, α-carbon traces, ribbon diagrams and electron density maps.

Suitable target MurG proteins and their associated binding sites to model using a method of the present invention include any MurG protein and binding sites that are at least in part structurally related to the *E. coli* MurG protein or its binding sites. A preferred target MurG structure that is at least in part structurally related includes a target MurG structure having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 36%, more preferably at least about 40%, even more preferablye at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80%, and more preferably at least about 90% identical to an amino acid sequence of the *E. coli* MurG protein, across the full-length of the target MurG structure sequence when using, for example, a sequence alignment program such as DNAsis ™ program (available from Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the GCγ™ program (available from the "GCγ", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs.

Preferred MurG proteins and their binding sites are set forth in the amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A,

CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. The amino acid sequences are publicly available.

A variety of MurG proteins from numerous organisms can be used to prepare models of MurG proteins and binding sites, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponoma pallidum.* It is noted that nucleotide and amino acid sequences for many of the above identified organisms are known and publicly available.

Preferred target MurG proteins and binding site structures to model also include, but are not limited to, derivatives of MurG proteins, such as a MurG protein having one or more amino acid residues substituted, deleted or added (referred to herein as MurG mutants), or proteins encoded by natural variants of a nucleic acid molecule encoding a MurG.

In another embodiment of the invention, the process of building a homology model for a protein is divided into the following steps:

(1) Determine which proteins are related to the model protein;

(2) Determine structurally conserved regions (SCRs);

(3) Align the amino acid sequence of the unknown protein with those of the reference protein(s) within the SCRs;

(4) Assign coordinates in the conserved regions;

(5) Predict conformations for the rest of the peptide chain, including loops between the SCRs and possibly the N- and C-termini;

(6) Search for the optimum side chain conformations for residues that differ from those in the reference proteins; and

(7) Use energy minimization and molecular dynamics to refine the molecular structure so that steric strain introduced during the model-building process can be relieved.

Published sequences are readily available through on-line databases on the Internet, such as SwissProt (http://www.expasy.ch/sprot/sprot-top.html). MurG specific and related sequences are obtained for use for building homology models by text-based or sequence similarity searching. SCRs for MurG is the entire protein, considering the E. coli MurG crystal structure is the only similar sequence with structural data. Alignment of the sequences using an appropriate alignment program and algorithm, such as Clustal W, allows appropriate assignment of the E. coli protein coordinates to a MurG sequence of unknown structure. The Modeler program performs the conformational predictions for the peptide chain and side chains. Dynamics and minimization using an appropriate program and algorithm, such as Discover.

Modeler Description:

Modeler is an automated homology-modeling scheme designed to find the most probable three-dimensional structure of a protein, given its amino acid sequence and its alignment with related structures. It derives 3D protein models without the time consuming separate stages of core region identification and loop region building or searching that is inherent to manual homology modeling schemes. The related or reference protein structures are used to derive spatial restraints expressed as probability density functions (PDFs) for each of the restrained features of the model. As an example, the main chain conformation of a given residue in the model will be described by restraints that depend upon the residue type, the main chain conformation of equivalent residues in the reference proteins and the local sequence similarity. The probability distribution functions that are used in restraining the model structure are derived from correlations between structural features in a database of families of homologous proteins aligned on the basis of their 3D structure. These functions are used to restrain C-C distances, main chain N--O distances, main chain and side chain dihedral angles, etc. The individual restraints are assembled into a single molecular probability density function (MPDF). The three-dimensional protein model is then obtained by an optimization of this MPDF. The optimization procedure itself consists of a variable target function method (Braun and Go, 1985) with conjugate gradient minimization scheme followed by an optional restrained simulated annealing molecular dynamics scheme.

While several reference structures are used in the traditional homology model building process, only one set of coordinates can be used in any one peptide segment. Modeler is able to simultaneously incorporate structural data from one or more reference proteins. Structural features in the reference proteins are used to derive spatial restraints which in turn are used to generate

model protein structures using conjugate gradient and simulated annealing optimization procedures.

Clustal W description:

Clustal W aligns multiple sequences using a progressive pairwise alignment algorithm. It first generates all possible pairwise alignments for a list of sequences and then builds the guide tree based on their pairwise sequence identity, aligning the sequences following the order of the guide tree. Several unique features in Clustal W improve the sensitivity of the alignment of divergent protein sequences (Thompson et al, 1994a).

(1) Individual weights are assigned to each sequence in a partial alignment in order to downweight near-duplicate sequences and upweight the most divergent ones.

(2) Amino acid substitution matrices are varied at different alignment stages according to the divergence of the sequences to be aligned.

(3) Residue-specific gap penalties and locally reduced gap penalties in hydrophilic regions encourage new gaps in potential loop regions rather than regular secondary structure.

(4) Positions in early alignments, where gaps have been opened, receive locally reduced gap penalties to encourage the opening of new gaps at these positions.

Discover Description:

The Discover program performs energy minimization, template forcing, torsion forcing, and dynamic trajectories and calculates properties such as interaction energies, derivatives, mean square displacements, and vibrational frequencies. It provides tools for performing simulations under various conditions including constant temperature, constant pressure, constant stress, periodic boundaries, and fixed and restrained atoms. Homology modeling methods are known to those skilled in the art and are described in the following homology references:

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All the references cited above are incorporated by reference in the entireties.

STRUCTURE BASED DRUG DESIGN

The present invention relates to the use of the crystal structure of the *E. coli* MurG protein represented by the atomic coordinates in Table 1 to make models of MurG proteins and binding sites

thereof. The present invention also relates to the use of the crystal structure, α-carbon backbone, α-carbon backbone plus conserved amino acid residue side chains or binding sites of the *E. coli* MurG protein to construct models of these structures in other MurG proteins.

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of MURG, in whole or in part.

On approach enabled by this invention, is to use the structure coordinates of MURG to design compounds that bind to the enzyme and alter the physical properties of the compounds in different ways, e.g., solubility. For example, this invention enables the design of compounds that act as inhibitors of the MURG enzyme by binding to, all or a portion of, the active site of MURG.

A second design approach is to probe a MurG crystal with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate MURG inhibitors and the enzyme. For example, high resolution Xray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their MURG inhibitor activity. Travis, J., Science, 262, p. 1374 (1993).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to MURG, with MURG. Thus, the time-dependent analysis of structural changes in MURG during its interaction with other molecules is enabled. The reaction intermediates of MURG can also be deduced from the reaction product in co-complex with MURG. Such information is useful to design improved analogues of known MURG inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the MURG enzyme and MURG-inhibitor co-complex. This provides a novel route for designing MURG inhibitors with both high specificity and stability.

Another approach made possible and enabled by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the MURG enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, E. C. et al., J. Coma. Chem., 13, pp. 505-524 (1992).

Because MURG may crystallize in more than one crystal form, the structure coordinates of MURG, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of MURG. They may also be used to solve the structure of

MURG mutants, MURG co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of MURG.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of MURG, a MurG mutant, or a MurG co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of MURG, may be determined using the MURG structure coordinates of this invention as provided in Tables 1-6. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

In addition, in accordance with this invention, MURG mutants may be crystallized in co-complex with known MURG inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type MURG. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information/provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between MURG and a chemical entity or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 2-3 .ANG. resolution X-ray date to an R value of about 0.20 or less using computer software, such as X-PLOR (Yale University, .COPYRGT.1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundel & Johnson, supra; Methods in Enzvmoloav, vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985). This information may thus be used to design, synthezie and optimize novel classes of MURG inhibitors.

The structure coordinates of MURG mutants provided in this invention also facilitate the identification of related proteins or enzymes analogous to MURG in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing UDP-glycosyltransferase mediated diseases.

The design of compounds that bind to or inhibit MURG according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with MURG. Non-covalent molecular interactions important in the association of MURG with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with MURG. Although certain portions of the compound will not directly participate in this association

with MURG, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of MURG, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with MURG.

The potential inhibitory or binding effect of a chemical compound on MURG may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and MURG, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to MURG and inhibit using the assay of Walker et al. patents (cited supra). In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of MURG may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of MURG.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with MURG and more particularly with the individual binding pockets of the MURG donor nucleotide binding site, acceptor binding site or membrane association site. This process may begin by visual inspection of, for example, the binding sites on the computer screen based on the MURG coordinates in Tables 1-6. Selected fragments or chemical entities may then be positioned tin a variety of orientations, or docked, within an individual binding pocket of MURG as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities, including but not limited to:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules" J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.

3. AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing" Proteins: Structure. Function, and Genetics, 8, pp. 195-202 (1990)) (AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.).

4. DOCK (Kuntz, 1. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions" J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of MURG. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include, but are not limited to:

1. CAVEAT (Bartlett, P. A. et al, "CAVEAT: A Program to Facilitate the Structure - Derived Design of Biologically Active Molecules". In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989)). CAVEAT is available from the University of California, Berkeley, Calif.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif). This area is reviewed in Martin, Y. C., "313 Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992)).

3. HOOK (available from Molecular Simulations, Burlington, Mass.).

Instead of proceeding to build a MurG inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other MURG binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include, but are not limited to:

1. LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. ComR. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, Calif.

2. LEGEND (Nishibata, Y. and A. Itai, Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, Mass.

3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to MURG may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as a MurG-inhibitor must also preferably traverse a volume not overlapping that occupied by the active site when it is bound to the native substrate. An effective MURG inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient MURG inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. MURG inhibitors may interact with the enzyme in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the enzyme.

A compound designed or selected as binding to MURG may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and chargedipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the enzyme when the inhibitor is bound to MURG, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include, but are not limited to: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. COPYRIGHT. 1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Francisco,

COPYRIGHT. 1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. COPYRIGHT. 1994]; and Insight II[Discover (Biosysm Technologies Inc., San Diego, Calif COPYRIGHT. 1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS Octane or IBM RISC/6000 workstation. Other hardware systems and software packages will be known to those skilled in the art.

Once a MurG-binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to MURG by the same computer methods described in detail, above.

COMPOUNDS AND COMPOSITIONS COMPRISING COMPOUNDS DERIVED FROM STRUCTURE BASED DRUG DESIGN

One embodiment of the present invention is a compound that is capable of binding to a MurG protein, inhibiting the activity of a MurG protein, or stimulating the activity of a MurG protein. Suitable inhibitory compounds of the present invention can: (1) inhibit (i.e., prevent or block) the activity of MurG enzyme by binding to a MurG donor nucleotide binding site and interfering with the binding of the donor nucleotide molecule; (2) inhibit the activity of MurG enzyme by binding to the MurG acceptor binding site and interfering with the binding of the acceptor molecule; (3) inhibit the activity of a MurG enzyme by binding to the membrane association site and interfering with the association of the protein with the bacterial membrane and/or acceptor molecule.

Another embodiment of the present invention is a compound that is capable of stimulating MurG activity. Suitable stimulatory compounds of the present invention can stimulate the activity of a MurG enzyme by binding to the protein at a binding site and causing an increase in enzymatic activity, for example, by increasing the enzymes affinity to bind a donor nucleotide, an acceptor molecule or improve the enzymes stability or increasing the binding affinity of a molecule to MurG.

Such compounds that bind to, inhibit or stimulate activity of a MurG protein include, for example, compounds that mimic donor nucleotide molecules. In preferred embodiments, the

compound includes, for example, pyrimidine nucleoside analogues. In yet another preferred embodiment, the compounds include compounds comprising a pyrimidine nucleoside with a substituent containing at least one heteroatom attached to the C5 hydroxyl. In more particular embodiments, pyrimidine derivatives make complementary hydrogen bonding contacts to the amide backbone segment containing Ile 245 and also contact glutamate 269.

Another embodiment of the present invention is a compound that binds to the acceptor binding site of the MurG protein, hereinafter referred to a acceptor analogs. An acceptor analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the acceptor binding site of a MurG protein. An acceptor analog, for example, is a compound that mimics the natural acceptor molecule, Lipid I. Examples of such acceptor analogs are set forth in Ha et al., J. Amer. Chem. Soc. 1999, and PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, incorporated herein by reference.

Another embodiment of the present invention is a compound that binds to the MurG protein, that are enzyme product analogs, hereinafter referred to as Lipid II analogs. A Lipid II analog refers to a compound that interacts with (i.e. , binds to, associates with, modifies) the acceptor binding site of a Mur G protein which mimics the product of the transglycosylase reaction.

Inhibitory and stimulatory compounds of the present invention can be identified by various means known to those of skill in the art. For example, binding of an inhibitory compound to, or otherwise interaction with, a MurG protein, can be determined with MurG in solution, for example, using assays described in PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, and PCT/US00/05554 , U.S. Provisional Application Nos. 60/122,966 and 60/137,696, incorporated herein by reference.

According to the present invention, suitable compounds of the present invention include peptides or other organic molecules, and inorganic molecules. Suitable organic molecules include small organic molecules. Preferably, a compound of the present invention is not harmful (i.e., toxic) to an animal when administered to an animal.

Compounds of the present invention also can be identified using structure based drug design techniques known to those skilled in the art and described herein above.

Also according to the present invention, compounds are suitable for use in the inhibition of bacterial or microbial growth in an animal, and for example, function as an antibiotic for treatment of bacterial infections in animals.

The present invention also includes compositions comprising compounds of the present invention that inhibit or stimulate MurG activity which function as antibiotics or antimicrobial agents in animals. Compositions of the present invention can be used therapeutically or diagnostically in an animal. Compositions of the present invention comprises at least one compound of the present invention. In a preferred embodiment, compositions of the present invention further comprise a carrier. More particularly, a suitable carrier is a pharmaceutically acceptable carrier known to those skilled in the art.

TABLE 1- ATOMIC COORDINATES OF E. COLI MURG PROTEIN

```
REMARK coordinates from minimization refinement
REMARK refinement resolution: 40.0 - 1.9 A
REMARK starting r= 0.2200 free_r= 0.2466
REMARK final    r= 0.2200 free_r= 0.2466
REMARK rmsd bonds= 0.005558  rmsd angles=  1.29505
REMARK wa= 1.08391
REMARK target= mlf cycles= 1 steps= 30
REMARK sg= P1 a= 60.613 b= 66.356 c= 67.902 alpha= 64.294 beta= 83.520 gamma= 65.448
REMARK parameter file 1  : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2  : CNS_TOPPAR:water_rep.param
REMARK parameter file 3  : CNS_TOPPAR:ion.param
REMARK molecular structure file: gen.mtf
REMARK input coordinates: gen.pdb
REMARK reflection file= native.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.9
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   0.747 B22=   2.098 B33=  -2.845
REMARK   B12=  -1.847 B13=  -3.752 B23=   6.401
REMARK B-factor correction applied to coordinate array B:     0.038
REMARK bulk solvent: density level= 0.351665 e/A^3, B-factor= 43.8282 A^2
REMARK reflections with |Fobs|/sigma_F < 2.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:     68102 (100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):   2825 (  4.1 % )
REMARK number of reflections rejected:                         3288 (  4.8 % )
REMARK total number of reflections used:                      61989 ( 91.0 % )
REMARK number of reflections in working set:                  55765 ( 81.9 % )
REMARK number of reflections in test set:                      6224 (  9.1 % )
CRYST1   60.613   66.356   67.902  64.29  83.52  65.45 P 1
REMARK FILENAME="minimize5.pdb"
REMARK DATE:14-Jan-00  15:25:36       created by user: sha
REMARK VERSION:0.5
ATOM      1  CB  LYS A   7       0.142   3.434  35.023  1.00 43.02      AAAA
ATOM      2  CG  LYS A   7       1.076   4.457  35.641  1.00 46.34      AAAA
ATOM      3  CD  LYS A   7       0.452   5.841  35.634  1.00 47.39      AAAA
ATOM      4  CE  LYS A   7       1.345   6.846  36.332  1.00 48.65      AAAA
ATOM      5  NZ  LYS A   7       0.780   8.221  36.276  1.00 51.04      AAAA
ATOM      6  C   LYS A   7      -2.239   2.733  34.833  1.00 39.64      AAAA
ATOM      7  O   LYS A   7      -2.050   1.717  34.160  1.00 39.64      AAAA
ATOM      8  N   LYS A   7      -0.974   2.320  36.947  1.00 42.05      AAAA
ATOM      9  CA  LYS A   7      -1.170   3.245  35.788  1.00 41.31      AAAA
ATOM     10  N   ARG A   8      -3.357   3.451  34.773  1.00 37.24      AAAA
```

	ATOM	11	CA	ARG	A	8	-4.469	3.076	33.906	1.00	34.91	AAAA
	ATOM	12	CB	ARG	A	8	-5.782	3.109	34.686	1.00	36.65	AAAA
	ATOM	13	CG	ARG	A	8	-5.950	2.017	35.721	1.00	39.89	AAAA
	ATOM	14	CD	ARG	A	8	-7.323	2.124	36.356	1.00	42.12	AAAA
	ATOM	15	NE	ARG	A	8	-7.663	0.960	37.163	1.00	45.03	AAAA
	ATOM	16	CZ	ARG	A	8	-7.031	0.610	38.279	1.00	46.29	AAAA
	ATOM	17	NH1	ARG	A	8	-6.015	1.337	38.725	1.00	46.88	AAAA
	ATOM	18	NH2	ARG	A	8	-7.420	-0.466	38.952	1.00	47.41	AAAA
	ATOM	19	C	ARG	A	8	-4.584	3.999	32.696	1.00	32.27	AAAA
	ATOM	20	O	ARG	A	8	-4.602	5.224	32.832	1.00	31.60	AAAA
	ATOM	21	N	LEU	A	9	-4.663	3.403	31.512	1.00	29.57	AAAA
	ATOM	22	CA	LEU	A	9	-4.792	4.171	30.283	1.00	27.45	AAAA
	ATOM	23	CB	LEU	A	9	-3.581	3.954	29.362	1.00	26.31	AAAA
	ATOM	24	CG	LEU	A	9	-3.752	4.466	27.916	1.00	25.77	AAAA
	ATOM	25	CD1	LEU	A	9	-3.670	5.985	27.895	1.00	24.31	AAAA
	ATOM	26	CD2	LEU	A	9	-2.679	3.870	26.993	1.00	26.22	AAAA
	ATOM	27	C	LEU	A	9	-6.038	3.762	29.523	1.00	25.97	AAAA
	ATOM	28	O	LEU	A	9	-6.397	2.587	29.485	1.00	25.57	AAAA
	ATOM	29	N	MET	A	10	-6.713	4.738	28.928	1.00	25.37	AAAA
	ATOM	30	CA	MET	A	10	-7.866	4.429	28.101	1.00	24.70	AAAA
	ATOM	31	CB	MET	A	10	-9.142	5.101	28.612	1.00	25.60	AAAA
	ATOM	32	CG	MET	A	10	-10.323	4.873	27.675	1.00	25.77	AAAA
	ATOM	33	SD	MET	A	10	-11.916	4.958	28.492	1.00	26.63	AAAA
	ATOM	34	CE	MET	A	10	-12.197	3.222	28.862	1.00	25.72	AAAA
	ATOM	35	C	MET	A	10	-7.528	4.943	26.715	1.00	23.31	AAAA
	ATOM	36	O	MET	A	10	-7.198	6.116	26.544	1.00	24.02	AAAA
	ATOM	37	N	VAL	A	11	-7.574	4.059	25.727	1.00	22.25	AAAA
	ATOM	38	CA	VAL	A	11	-7.278	4.461	24.359	1.00	22.34	AAAA
	ATOM	39	CB	VAL	A	11	-6.444	3.386	23.624	1.00	22.75	AAAA
	ATOM	40	CG1	VAL	A	11	-6.256	3.768	22.158	1.00	20.51	AAAA
	ATOM	41	CG2	VAL	A	11	-5.082	3.239	24.310	1.00	21.75	AAAA
	ATOM	42	C	VAL	A	11	-8.612	4.654	23.646	1.00	22.94	AAAA
	ATOM	43	O	VAL	A	11	-9.525	3.843	23.804	1.00	23.37	AAAA
	ATOM	44	N	MET	A	12	-8.722	5.734	22.878	1.00	22.18	AAAA
	ATOM	45	CA	MET	A	12	-9.949	6.034	22.146	1.00	23.10	AAAA
	ATOM	46	CB	MET	A	12	-10.496	7.399	22.589	1.00	22.78	AAAA
	ATOM	47	CG	MET	A	12	-10.359	7.655	24.096	1.00	23.92	AAAA
	ATOM	48	SD	MET	A	12	-10.955	9.279	24.657	1.00	25.51	AAAA
	ATOM	49	CE	MET	A	12	-9.641	10.349	24.162	1.00	22.79	AAAA
	ATOM	50	C	MET	A	12	-9.582	6.072	20.673	1.00	22.97	AAAA
	ATOM	51	O	MET	A	12	-8.917	6.997	20.226	1.00	21.16	AAAA
	ATOM	52	N	ALA	A	13	-9.992	5.057	19.921	1.00	26.97	AAAA
	ATOM	53	CA	ALA	A	13	-9.665	5.008	18.498	1.00	30.88	AAAA
	ATOM	54	CB	ALA	A	13	-8.381	4.212	18.288	1.00	31.18	AAAA
	ATOM	55	C	ALA	A	13	-10.813	4.412	17.685	1.00	34.35	AAAA

	ATOM	56	O	ALA	A	13	-11.328	3.335	18.006	1.00	35.86	AAAA
	ATOM	57	N	GLY	A	14	-11.176	5.127	16.622	1.00	37.37	AAAA
	ATOM	58	CA	GLY	A	14	-12.287	4.762	15.757	1.00	40.54	AAAA
	ATOM	59	C	GLY	A	14	-12.239	3.583	14.808	1.00	41.52	AAAA
	ATOM	60	O	GLY	A	14	-11.267	2.831	14.755	1.00	43.26	AAAA
	ATOM	61	N	GLY	A	15	-13.322	3.451	14.042	1.00	42.70	AAAA
	ATOM	62	CA	GLY	A	15	-13.491	2.363	13.094	1.00	43.13	AAAA
	ATOM	63	C	GLY	A	15	-12.660	2.286	11.825	1.00	43.41	AAAA
	ATOM	64	O	GLY	A	15	-13.212	2.187	10.730	1.00	44.39	AAAA
	ATOM	65	N	THR	A	16	-11.340	2.333	11.966	1.00	43.38	AAAA
	ATOM	66	CA	THR	A	16	-10.426	2.204	10.833	1.00	43.22	AAAA
	ATOM	67	CB	THR	A	16	-10.120	3.551	10.110	1.00	44.23	AAAA
	ATOM	68	OG1	THR	A	16	-9.302	4.375	10.949	1.00	44.41	AAAA
	ATOM	69	CG2	THR	A	16	-11.404	4.286	9.754	1.00	43.74	AAAA
	ATOM	70	C	THR	A	16	-9.118	1.679	11.402	1.00	43.06	AAAA
	ATOM	71	O	THR	A	16	-8.728	2.042	12.517	1.00	42.99	AAAA
	ATOM	72	N	GLY	A	17	-8.453	0.810	10.649	1.00	41.81	AAAA
	ATOM	73	CA	GLY	A	17	-7.190	0.268	11.109	1.00	40.71	AAAA
	ATOM	74	C	GLY	A	17	-6.202	1.401	11.275	1.00	39.54	AAAA
	ATOM	75	O	GLY	A	17	-5.275	1.330	12.085	1.00	39.73	AAAA
	ATOM	76	N	GLY	A	18	-6.413	2.460	10.500	1.00	37.79	AAAA
	ATOM	77	CA	GLY	A	18	-5.539	3.611	10.572	1.00	35.68	AAAA
	ATOM	78	C	GLY	A	18	-5.394	4.116	11.994	1.00	34.88	AAAA
	ATOM	79	O	GLY	A	18	-4.285	4.441	12.427	1.00	35.21	AAAA
	ATOM	80	N	HIS	A	19	-6.503	4.186	12.728	1.00	32.89	AAAA
	ATOM	81	CA	HIS	A	19	-6.454	4.664	14.110	1.00	32.14	AAAA
	ATOM	82	CB	HIS	A	19	-7.759	5.371	14.504	1.00	30.28	AAAA
	ATOM	83	CG	HIS	A	19	-8.150	6.504	13.605	1.00	28.85	AAAA
	ATOM	84	CD2	HIS	A	19	-9.336	6.808	13.027	1.00	27.83	AAAA
	ATOM	85	ND1	HIS	A	19	-7.288	7.524	13.265	1.00	28.68	AAAA
	ATOM	86	CE1	HIS	A	19	-7.926	8.407	12.517	1.00	28.09	AAAA
	ATOM	87	NE2	HIS	A	19	-9.170	7.996	12.358	1.00	27.45	AAAA
	ATOM	88	C	HIS	A	19	-6.229	3.533	15.108	1.00	31.91	AAAA
	ATOM	89	O	HIS	A	19	-5.480	3.684	16.072	1.00	31.76	AAAA
	ATOM	90	N	VAL	A	20	-6.895	2.407	14.881	1.00	31.82	AAAA
	ATOM	91	CA	VAL	A	20	-6.813	1.271	15.788	1.00	33.08	AAAA
	ATOM	92	CB	VAL	A	20	-7.875	0.215	15.430	1.00	33.31	AAAA
	ATOM	93	CG1	VAL	A	20	-7.766	-0.982	16.361	1.00	33.91	AAAA
	ATOM	94	CG2	VAL	A	20	-9.260	0.830	15.540	1.00	34.25	AAAA
	ATOM	95	C	VAL	A	20	-5.452	0.587	15.898	1.00	33.31	AAAA
	ATOM	96	O	VAL	A	20	-4.977	0.337	17.008	1.00	32.99	AAAA
	ATOM	97	N	PHE	A	21	-4.823	0.288	14.765	1.00	33.64	AAAA
	ATOM	98	CA	PHE	A	21	-3.526	-0.385	14.794	1.00	33.68	AAAA
	ATOM	99	CB	PHE	A	21	-3.020	-0.648	13.368	1.00	35.58	AAAA
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	ATOM	310	OE2	GLU	A	47	-14.995	1.652	17.350	1.00	32.08	AAAA
	ATOM	311	C	GLU	A	47	-13.225	-3.123	17.972	1.00	36.96	AAAA
	ATOM	312	O	GLU	A	47	-12.612	-3.744	18.842	1.00	37.00	AAAA
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	ATOM	314	CA	ALA	A	48	-15.342	-4.066	18.700	1.00	36.98	AAAA
	ATOM	315	CB	ALA	A	48	-16.823	-3.917	18.365	1.00	37.33	AAAA
	ATOM	316	C	ALA	A	48	-14.943	-5.533	18.623	1.00	38.23	AAAA
	ATOM	317	O	ALA	A	48	-15.100	-6.281	19.590	1.00	37.91	AAAA
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	ATOM	320	CB	ASP	A	49	-14.477	-7.832	15.909	1.00	42.68	AAAA
	ATOM	321	CG	ASP	A	49	-15.988	-7.912	15.783	1.00	44.91	AAAA
	ATOM	322	OD1	ASP	A	49	-16.612	-8.681	16.549	1.00	45.64	AAAA
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	ATOM	324	C	ASP	A	49	-12.524	-7.519	17.426	1.00	40.10	AAAA
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ATOM	517	O	LEU	A	74	-23.768	16.012	18.206	1.00	37.74	AAAA
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ATOM	519	CA	ILE	A	75	-21.923	17.975	17.678	1.00	39.02	AAAA
ATOM	520	CB	ILE	A	75	-20.605	18.707	17.319	1.00	40.76	AAAA
ATOM	521	CG2	ILE	A	75	-20.616	19.109	15.856	1.00	41.16	AAAA
ATOM	522	CG1	ILE	A	75	-20.426	19.938	18.209	1.00	42.50	AAAA
ATOM	523	CD1	ILE	A	75	-20.302	19.616	19.690	1.00	44.15	AAAA
ATOM	524	C	ILE	A	75	-23.114	18.886	17.377	1.00	38.41	AAAA
ATOM	525	O	ILE	A	75	-23.396	19.818	18.130	1.00	38.12	AAAA
ATOM	526	N	ALA	A	76	-23.816	18.602	16.283	1.00	38.04	AAAA
ATOM	527	CA	ALA	A	76	-24.971	19.399	15.878	1.00	37.19	AAAA
ATOM	528	CB	ALA	A	76	-25.060	19.454	14.350	1.00	37.36	AAAA
ATOM	529	C	ALA	A	76	-26.268	18.847	16.455	1.00	36.15	AAAA
ATOM	530	O	ALA	A	76	-27.352	19.323	16.124	1.00	35.97	AAAA
ATOM	531	N	ALA	A	77	-26.156	17.834	17.309	1.00	34.42	AAAA
ATOM	532	CA	ALA	A	77	-27.326	17.225	17.935	1.00	33.14	AAAA
ATOM	533	CB	ALA	A	77	-27.460	15.780	17.499	1.00	33.13	AAAA
ATOM	534	C	ALA	A	77	-27.125	17.311	19.443	1.00	32.59	AAAA
ATOM	535	O	ALA	A	77	-26.502	16.436	20.042	1.00	31.09	AAAA
ATOM	536	N	PRO	A	78	-27.664	18.372	20.073	1.00	32.06	AAAA
ATOM	537	CD	PRO	A	78	-28.619	19.290	19.423	1.00	31.98	AAAA
ATOM	538	CA	PRO	A	78	-27.577	18.653	21.514	1.00	31.07	AAAA
ATOM	539	CB	PRO	A	78	-28.671	19.701	21.727	1.00	32.32	AAAA
ATOM	540	CG	PRO	A	78	-28.703	20.427	20.414	1.00	32.04	AAAA
ATOM	541	C	PRO	A	78	-27.748	17.450	22.443	1.00	30.50	AAAA
ATOM	542	O	PRO	A	78	-26.874	17.155	23.257	1.00	29.52	AAAA
ATOM	543	N	LEU	A	79	-28.878	16.766	22.334	1.00	28.95	AAAA
ATOM	544	CA	LEU	A	79	-29.130	15.619	23.194	1.00	29.33	AAAA
ATOM	545	CB	LEU	A	79	-30.573	15.137	23.023	1.00	29.48	AAAA
ATOM	546	CG	LEU	A	79	-31.644	16.154	23.435	1.00	30.82	AAAA
ATOM	547	CD1	LEU	A	79	-33.025	15.542	23.234	1.00	31.23	AAAA
ATOM	548	CD2	LEU	A	79	-31.450	16.558	24.901	1.00	30.46	AAAA
ATOM	549	C	LEU	A	79	-28.160	14.465	22.950	1.00	28.58	AAAA
ATOM	550	O	LEU	A	79	-27.745	13.795	23.898	1.00	27.00	AAAA

ATOM	551	N	ARG	A	80	-27.794	14.240	21.689	1.00	27.70	AAAA
ATOM	552	CA	ARG	A	80	-26.877	13.156	21.348	1.00	28.33	AAAA
ATOM	553	CB	ARG	A	80	-26.813	12.941	19.836	1.00	30.44	AAAA
ATOM	554	CG	ARG	A	80	-28.037	12.294	19.222	1.00	36.59	AAAA
ATOM	555	CD	ARG	A	80	-27.657	11.616	17.915	1.00	38.91	AAAA
ATOM	556	NE	ARG	A	80	-28.821	11.189	17.151	1.00	43.51	AAAA
ATOM	557	CZ	ARG	A	80	-29.537	11.991	16.370	1.00	44.36	AAAA
ATOM	558	NH1	ARG	A	80	-29.207	13.270	16.244	1.00	45.19	AAAA
ATOM	559	NH2	ARG	A	80	-30.589	11.513	15.721	1.00	45.91	AAAA
ATOM	560	C	ARG	A	80	-25.464	13.384	21.871	1.00	27.39	AAAA
ATOM	561	O	ARG	A	80	-24.835	12.455	22.392	1.00	26.07	AAAA
ATOM	562	N	ILE	A	81	-24.950	14.603	21.719	1.00	26.19	AAAA
ATOM	563	CA	ILE	A	81	-23.608	14.886	22.217	1.00	24.89	AAAA
ATOM	564	CB	ILE	A	81	-23.081	16.269	21.702	1.00	25.72	AAAA
ATOM	565	CG2	ILE	A	81	-24.069	17.373	22.021	1.00	26.90	AAAA
ATOM	566	CG1	ILE	A	81	-21.722	16.584	22.332	1.00	25.98	AAAA
ATOM	567	CD1	ILE	A	81	-20.696	15.474	22.169	1.00	26.39	AAAA
ATOM	568	C	ILE	A	81	-23.609	14.832	23.752	1.00	24.30	AAAA
ATOM	569	O	ILE	A	81	-22.669	14.315	24.365	1.00	22.57	AAAA
ATOM	570	N	PHE	A	82	-24.672	15.344	24.367	1.00	22.71	AAAA
ATOM	571	CA	PHE	A	82	-24.800	15.333	25.827	1.00	22.28	AAAA
ATOM	572	CB	PHE	A	82	-26.099	16.029	26.236	1.00	21.54	AAAA
ATOM	573	CG	PHE	A	82	-26.281	16.184	27.730	1.00	20.67	AAAA
ATOM	574	CD1	PHE	A	82	-25.244	16.644	28.538	1.00	21.08	AAAA
ATOM	575	CD2	PHE	A	82	-27.512	15.907	28.318	1.00	21.44	AAAA
ATOM	576	CE1	PHE	A	82	-25.430	16.831	29.916	1.00	20.18	AAAA
ATOM	577	CE2	PHE	A	82	-27.719	16.093	29.700	1.00	19.77	AAAA
ATOM	578	CZ	PHE	A	82	-26.678	16.555	30.497	1.00	20.80	AAAA
ATOM	579	C	PHE	A	82	-24.797	13.887	26.330	1.00	21.61	AAAA
ATOM	580	O	PHE	A	82	-24.091	13.536	27.285	1.00	21.05	AAAA
ATOM	581	N	ASN	A	83	-25.577	13.042	25.669	1.00	21.80	AAAA
ATOM	582	CA	ASN	A	83	-25.648	11.640	26.045	1.00	22.62	AAAA
ATOM	583	CB	ASN	A	83	-26.806	10.969	25.296	1.00	22.62	AAAA
ATOM	584	CG	ASN	A	83	-26.921	9.495	25.612	1.00	25.00	AAAA
ATOM	585	OD1	ASN	A	83	-26.227	8.677	25.031	1.00	26.80	AAAA
ATOM	586	ND2	ASN	A	83	-27.791	9.153	26.548	1.00	28.27	AAAA
ATOM	587	C	ASN	A	83	-24.324	10.888	25.805	1.00	21.61	AAAA
ATOM	588	O	ASN	A	83	-23.903	10.080	26.639	1.00	22.04	AAAA
ATOM	589	N	ALA	A	84	-23.658	11.150	24.686	1.00	19.98	AAAA
ATOM	590	CA	ALA	A	84	-22.383	10.480	24.401	1.00	19.25	AAAA
ATOM	591	CB	ALA	A	84	-21.912	10.817	22.981	1.00	20.79	AAAA
ATOM	592	C	ALA	A	84	-21.318	10.906	25.424	1.00	19.48	AAAA
ATOM	593	O	ALA	A	84	-20.509	10.095	25.880	1.00	18.26	AAAA
ATOM	594	N	TRP	A	85	-21.322	12.188	25.769	1.00	17.57	AAAA
ATOM	595	CA	TRP	A	85	-20.390	12.736	26.749	1.00	18.15	AAAA

ATOM	596	CB	TRP	A	85	-20.561	14.260	26.781	1.00	17.16	AAAA
ATOM	597	CG	TRP	A	85	-19.863	15.007	27.892	1.00	16.32	AAAA
ATOM	598	CD2	TRP	A	85	-20.300	16.233	28.472	1.00	16.29	AAAA
ATOM	599	CE2	TRP	A	85	-19.340	16.605	29.445	1.00	15.39	AAAA
ATOM	600	CE3	TRP	A	85	-21.413	17.062	28.266	1.00	16.28	AAAA
ATOM	601	CD1	TRP	A	85	-18.677	14.682	28.519	1.00	15.58	AAAA
ATOM	602	NE1	TRP	A	85	-18.364	15.639	29.454	1.00	14.76	AAAA
ATOM	603	CZ2	TRP	A	85	-19.458	17.762	30.204	1.00	14.50	AAAA
ATOM	604	CZ3	TRP	A	85	-21.530	18.218	29.027	1.00	16.55	AAAA
ATOM	605	CH2	TRP	A	85	-20.553	18.558	29.988	1.00	15.65	AAAA
ATOM	606	C	TRP	A	85	-20.639	12.099	28.125	1.00	19.04	AAAA
ATOM	607	O	TRP	A	85	-19.696	11.691	28.820	1.00	17.64	AAAA
ATOM	608	N	ARG	A	86	-21.903	11.986	28.516	1.00	18.52	AAAA
ATOM	609	CA	ARG	A	86	-22.216	11.375	29.803	1.00	19.34	AAAA
ATOM	610	CB	ARG	A	86	-23.675	11.654	30.181	1.00	19.24	AAAA
ATOM	611	CG	ARG	A	86	-23.892	13.104	30.660	1.00	18.36	AAAA
ATOM	612	CD	ARG	A	86	-25.318	13.357	31.154	1.00	19.61	AAAA
ATOM	613	NE	ARG	A	86	-26.303	13.245	30.072	1.00	19.64	AAAA
ATOM	614	CZ	ARG	A	86	-27.021	12.156	29.807	1.00	21.06	AAAA
ATOM	615	NH1	ARG	A	86	-26.880	11.063	30.548	1.00	19.09	AAAA
ATOM	616	NH2	ARG	A	86	-27.879	12.156	28.787	1.00	18.59	AAAA
ATOM	617	C	ARG	A	86	-21.910	9.870	29.815	1.00	20.22	AAAA
ATOM	618	O	ARG	A	86	-21.520	9.319	30.845	1.00	20.88	AAAA
ATOM	619	N	GLN	A	87	-22.076	9.202	28.681	1.00	19.83	AAAA
ATOM	620	CA	GLN	A	87	-21.764	7.776	28.607	1.00	20.57	AAAA
ATOM	621	CB	GLN	A	87	-22.100	7.210	27.230	1.00	20.73	AAAA
ATOM	622	CG	GLN	A	87	-23.568	6.907	26.979	1.00	22.18	AAAA
ATOM	623	CD	GLN	A	87	-23.779	6.329	25.590	1.00	23.54	AAAA
ATOM	624	OE1	GLN	A	87	-23.193	5.308	25.234	1.00	24.56	AAAA
ATOM	625	NE2	GLN	A	87	-24.614	6.982	24.797	1.00	23.56	AAAA
ATOM	626	C	GLN	A	87	-20.268	7.599	28.859	1.00	20.58	AAAA
ATOM	627	O	GLN	A	87	-19.846	6.687	29.576	1.00	18.93	AAAA
ATOM	628	N	ALA	A	88	-19.471	8.479	28.255	1.00	20.24	AAAA
ATOM	629	CA	ALA	A	88	-18.023	8.436	28.412	1.00	20.23	AAAA
ATOM	630	CB	ALA	A	88	-17.355	9.386	27.419	1.00	18.84	AAAA
ATOM	631	C	ALA	A	88	-17.622	8.787	29.841	1.00	20.11	AAAA
ATOM	632	O	ALA	A	88	-16.687	8.202	30.388	1.00	20.39	AAAA
ATOM	633	N	ARG	A	89	-18.309	9.745	30.454	1.00	18.15	AAAA
ATOM	634	CA	ARG	A	89	-17.985	10.091	31.836	1.00	19.16	AAAA
ATOM	635	CB	ARG	A	89	-18.797	11.302	32.313	1.00	16.58	AAAA
ATOM	636	CG	ARG	A	89	-18.225	12.657	31.896	1.00	17.41	AAAA
ATOM	637	CD	ARG	A	89	-19.196	13.769	32.284	1.00	15.10	AAAA
ATOM	638	NE	ARG	A	89	-19.437	13.835	33.729	1.00	16.60	AAAA
ATOM	639	CZ	ARG	A	89	-18.675	14.506	34.587	1.00	16.76	AAAA
ATOM	640	NH1	ARG	A	89	-17.609	15.173	34.157	1.00	16.02	AAAA

ATOM	641	NH2	ARG	A	89	-18.990	14.531	35.877	1.00	15.64	AAAA
ATOM	642	C	ARG	A	89	-18.258	8.902	32.764	1.00	19.91	AAAA
ATOM	643	O	ARG	A	89	-17.469	8.618	33.674	1.00	18.92	AAAA
ATOM	644	N	ALA	A	90	-19.371	8.213	32.544	1.00	21.12	AAAA
ATOM	645	CA	ALA	A	90	-19.719	7.063	33.386	1.00	23.31	AAAA
ATOM	646	CB	ALA	A	90	-21.080	6.502	32.976	1.00	24.02	AAAA
ATOM	647	C	ALA	A	90	-18.640	5.990	33.257	1.00	24.57	AAAA
ATOM	648	O	ALA	A	90	-18.236	5.367	34.243	1.00	24.35	AAAA
ATOM	649	N	ILE	A	91	-18.173	5.790	32.031	1.00	24.03	AAAA
ATOM	650	CA	ILE	A	91	-17.135	4.816	31.746	1.00	24.73	AAAA
ATOM	651	CB	ILE	A	91	-16.922	4.699	30.209	1.00	25.99	AAAA
ATOM	652	CG2	ILE	A	91	-15.547	4.086	29.890	1.00	25.27	AAAA
ATOM	653	CG1	ILE	A	91	-18.061	3.875	29.601	1.00	25.74	AAAA
ATOM	654	CD1	ILE	A	91	-18.123	3.931	28.085	1.00	25.37	AAAA
ATOM	655	C	ILE	A	91	-15.823	5.196	32.436	1.00	25.69	AAAA
ATOM	656	O	ILE	A	91	-15.133	4.339	32.991	1.00	25.17	AAAA
ATOM	657	N	MET	A	92	-15.482	6.481	32.410	1.00	24.39	AAAA
ATOM	658	CA	MET	A	92	-14.243	6.933	33.024	1.00	24.61	AAAA
ATOM	659	CB	MET	A	92	-13.798	8.258	32.391	1.00	23.19	AAAA
ATOM	660	CG	MET	A	92	-13.480	8.088	30.908	1.00	21.54	AAAA
ATOM	661	SD	MET	A	92	-12.816	9.554	30.108	1.00	21.51	AAAA
ATOM	662	CE	MET	A	92	-12.756	9.008	28.463	1.00	17.14	AAAA
ATOM	663	C	MET	A	92	-14.325	7.041	34.545	1.00	24.72	AAAA
ATOM	664	O	MET	A	92	-13.311	6.918	35.236	1.00	24.71	AAAA
ATOM	665	N	LYS	A	93	-15.524	7.262	35.070	1.00	24.64	AAAA
ATOM	666	CA	LYS	A	93	-15.700	7.337	36.517	1.00	26.89	AAAA
ATOM	667	CB	LYS	A	93	-17.102	7.840	36.864	1.00	27.06	AAAA
ATOM	668	CG	LYS	A	93	-17.269	9.345	36.831	1.00	26.10	AAAA
ATOM	669	CD	LYS	A	93	-18.641	9.742	37.366	1.00	28.56	AAAA
ATOM	670	CE	LYS	A	93	-18.762	11.251	37.483	1.00	28.03	AAAA
ATOM	671	NZ	LYS	A	93	-20.068	11.663	38.060	1.00	29.77	AAAA
ATOM	672	C	LYS	A	93	-15.495	5.938	37.119	1.00	28.19	AAAA
ATOM	673	O	LYS	A	93	-14.994	5.792	38.238	1.00	28.43	AAAA
ATOM	674	N	ALA	A	94	-15.880	4.912	36.367	1.00	29.30	AAAA
ATOM	675	CA	ALA	A	94	-15.736	3.532	36.831	1.00	30.63	AAAA
ATOM	676	CB	ALA	A	94	-16.750	2.635	36.131	1.00	30.03	AAAA
ATOM	677	C	ALA	A	94	-14.325	2.981	36.622	1.00	30.40	AAAA
ATOM	678	O	ALA	A	94	-13.778	2.322	37.507	1.00	30.67	AAAA
ATOM	679	N	TYR	A	95	-13.735	3.255	35.462	1.00	29.39	AAAA
ATOM	680	CA	TYR	A	95	-12.394	2.764	35.163	1.00	29.94	AAAA
ATOM	681	CB	TYR	A	95	-12.189	2.685	33.648	1.00	29.85	AAAA
ATOM	682	CG	TYR	A	95	-10.838	2.151	33.224	1.00	31.64	AAAA
ATOM	683	CD1	TYR	A	95	-10.382	0.907	33.669	1.00	31.90	AAAA
ATOM	684	CE1	TYR	A	95	-9.139	0.414	33.270	1.00	32.14	AAAA
ATOM	685	CD2	TYR	A	95	-10.015	2.886	32.370	1.00	30.90	AAAA

ATOM	686	CE2	TYR	A	95	-8.779	2.405	31.969	1.00	31.95	AAAA
ATOM	687	CZ	TYR	A	95	-8.345	1.167	32.423	1.00	32.95	AAAA
ATOM	688	OH	TYR	A	95	-7.120	0.687	32.019	1.00	33.09	AAAA
ATOM	689	C	TYR	A	95	-11.312	3.633	35.791	1.00	29.90	AAAA
ATOM	690	O	TYR	A	95	-10.253	3.137	36.190	1.00	28.99	AAAA
ATOM	691	N	LYS	A	96	-11.584	4.930	35.871	1.00	28.94	AAAA
ATOM	692	CA	LYS	A	96	-10.658	5.893	36.452	1.00	29.17	AAAA
ATOM	693	CB	LYS	A	96	-10.543	5.658	37.966	1.00	32.14	AAAA
ATOM	694	CG	LYS	A	96	-11.871	5.829	38.690	1.00	35.57	AAAA
ATOM	695	CD	LYS	A	96	-11.784	5.541	40.183	1.00	38.37	AAAA
ATOM	696	CE	LYS	A	96	-13.158	5.718	40.828	1.00	39.96	AAAA
ATOM	697	NZ	LYS	A	96	-13.170	5.428	42.295	1.00	42.96	AAAA
ATOM	698	C	LYS	A	96	-9.274	5.884	35.817	1.00	27.78	AAAA
ATOM	699	O	LYS	A	96	-8.281	5.608	36.482	1.00	28.12	AAAA
ATOM	700	N	PRO	A	97	-9.187	6.185	34.509	1.00	26.15	AAAA
ATOM	701	CD	PRO	A	97	-10.258	6.519	33.547	1.00	24.76	AAAA
ATOM	702	CA	PRO	A	97	-7.867	6.191	33.868	1.00	24.70	AAAA
ATOM	703	CB	PRO	A	97	-8.202	6.241	32.381	1.00	23.96	AAAA
ATOM	704	CG	PRO	A	97	-9.477	7.078	32.362	1.00	24.55	AAAA
ATOM	705	C	PRO	A	97	-7.060	7.408	34.320	1.00	24.77	AAAA
ATOM	706	O	PRO	A	97	-7.628	8.438	34.684	1.00	23.93	AAAA
ATOM	707	N	ASP	A	98	-5.737	7.288	34.314	1.00	24.94	AAAA
ATOM	708	CA	ASP	A	98	-4.890	8.404	34.717	1.00	24.75	AAAA
ATOM	709	CB	ASP	A	98	-3.554	7.891	35.261	1.00	26.69	AAAA
ATOM	710	CG	ASP	A	98	-3.725	7.040	36.509	1.00	28.25	AAAA
ATOM	711	OD1	ASP	A	98	-3.546	5.808	36.426	1.00	28.34	AAAA
ATOM	712	OD2	ASP	A	98	-4.053	7.603	37.569	1.00	29.50	AAAA
ATOM	713	C	ASP	A	98	-4.654	9.328	33.529	1.00	23.89	AAAA
ATOM	714	O	ASP	A	98	-4.267	10.486	33.681	1.00	22.57	AAAA
ATOM	715	N	VAL	A	99	-4.918	8.807	32.339	1.00	24.10	AAAA
ATOM	716	CA	VAL	A	99	-4.740	9.569	31.111	1.00	23.85	AAAA
ATOM	717	CB	VAL	A	99	-3.237	9.633	30.730	1.00	25.11	AAAA
ATOM	718	CG1	VAL	A	99	-2.684	8.220	30.614	1.00	25.72	AAAA
ATOM	719	CG2	VAL	A	99	-3.044	10.372	29.420	1.00	24.76	AAAA
ATOM	720	C	VAL	A	99	-5.498	8.865	29.989	1.00	22.90	AAAA
ATOM	721	O	VAL	A	99	-5.767	7.667	30.073	1.00	22.05	AAAA
ATOM	722	N	VAL	A	100	-5.869	9.613	28.951	1.00	22.07	AAAA
ATOM	723	CA	VAL	A	100	-6.544	9.008	27.808	1.00	21.38	AAAA
ATOM	724	CB	VAL	A	100	-8.038	9.451	27.663	1.00	21.17	AAAA
ATOM	725	CG1	VAL	A	100	-8.804	9.095	28.914	1.00	21.06	AAAA
ATOM	726	CG2	VAL	A	100	-8.139	10.942	27.354	1.00	22.14	AAAA
ATOM	727	C	VAL	A	100	-5.777	9.398	26.559	1.00	21.31	AAAA
ATOM	728	O	VAL	A	100	-5.244	10.505	26.464	1.00	21.01	AAAA
ATOM	729	N	LEU	A	101	-5.701	8.468	25.612	1.00	21.54	AAAA
ATOM	730	CA	LEU	A	101	-4.994	8.697	24.362	1.00	22.01	AAAA

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	ATOM	733	CD1	LEU	A	101	-2.230	6.515	22.696	1.00	25.87	AAAA
	ATOM	734	CD2	LEU	A	101	-2.930	8.854	22.187	1.00	26.43	AAAA
	ATOM	735	C	LEU	A	101	-6.006	8.644	23.222	1.00	21.51	AAAA
	ATOM	736	O	LEU	A	101	-6.667	7.625	23.029	1.00	21.94	AAAA
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	ATOM	760	CG	TYR	A	106	-17.536	9.257	15.303	1.00	33.49	AAAA
	ATOM	761	CD1	TYR	A	106	-18.269	8.802	16.400	1.00	34.81	AAAA
	ATOM	762	CE1	TYR	A	106	-19.038	7.634	16.323	1.00	36.18	AAAA
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	ATOM	774	C	VAL	A	107	-14.836	8.993	20.223	1.00	23.22	AAAA
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ATOM	791	C	PRO	A	110	-16.136	12.031	24.524	1.00	18.52	AAAA
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ATOM	817	C	ALA	A	115	-11.506	14.530	30.693	1.00	16.10	AAAA
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ATOM	830	CH2	TRP	A	116	-13.072	22.834	28.439	1.00	25.35	AAAA
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	ATOM	1153	CA	GLY	A	160	5.727	9.628	13.075	1.00	29.63	AAAA
	ATOM	1154	C	GLY	A	160	4.678	8.608	13.483	1.00	29.61	AAAA
	ATOM	1155	O	GLY	A	160	3.917	8.849	14.416	1.00	29.30	AAAA
	ATOM	1156	N	ASN	A	161	4.635	7.475	12.782	1.00	29.30	AAAA
	ATOM	1157	CA	ASN	A	161	3.677	6.401	13.074	1.00	29.78	AAAA
	ATOM	1158	CB	ASN	A	161	2.800	6.097	11.858	1.00	30.70	AAAA
	ATOM	1159	CG	ASN	A	161	1.755	7.154	11.609	1.00	32.16	AAAA
	ATOM	1160	OD1	ASN	A	161	0.951	7.461	12.492	1.00	31.78	AAAA
	ATOM	1161	ND2	ASN	A	161	1.750	7.711	10.400	1.00	30.88	AAAA
	ATOM	1162	C	ASN	A	161	4.344	5.089	13.462	1.00	29.50	AAAA
	ATOM	1163	O	ASN	A	161	5.471	4.810	13.058	1.00	29.61	AAAA
	ATOM	1164	N	PRO	A	162	3.648	4.263	14.251	1.00	29.59	AAAA
	ATOM	1165	CD	PRO	A	162	2.441	4.571	15.039	1.00	29.95	AAAA
	ATOM	1166	CA	PRO	A	162	4.219	2.977	14.650	1.00	29.65	AAAA
	ATOM	1167	CB	PRO	A	162	3.143	2.389	15.553	1.00	29.79	AAAA
	ATOM	1168	CG	PRO	A	162	2.559	3.608	16.200	1.00	30.38	AAAA
	ATOM	1169	C	PRO	A	162	4.423	2.135	13.389	1.00	30.13	AAAA
	ATOM	1170	O	PRO	A	162	3.535	2.063	12.531	1.00	28.48	AAAA
	ATOM	1171	N	VAL	A	163	5.590	1.508	13.287	1.00	29.92	AAAA
	ATOM	1172	CA	VAL	A	163	5.935	0.664	12.149	1.00	29.89	AAAA
	ATOM	1173	CB	VAL	A	163	7.182	1.224	11.417	1.00	31.04	AAAA
	ATOM	1174	CG1	VAL	A	163	7.571	0.308	10.260	1.00	30.44	AAAA
	ATOM	1175	CG2	VAL	A	163	6.902	2.631	10.914	1.00	29.10	AAAA
	ATOM	1176	C	VAL	A	163	6.258	-0.744	12.652	1.00	31.06	AAAA
	ATOM	1177	O	VAL	A	163	6.884	-0.892	13.706	1.00	29.66	AAAA
	ATOM	1178	N	ARG	A	164	5.820	-1.773	11.927	1.00	31.83	AAAA
	ATOM	1179	CA	ARG	A	164	6.124	-3.142	12.339	1.00	34.34	AAAA
	ATOM	1180	CB	ARG	A	164	5.533	-4.167	11.354	1.00	36.31	AAAA

	ATOM	1181	CG	ARG	A	164	5.704	-3.841	9.876	1.00	39.86	AAAA
	ATOM	1182	CD	ARG	A	164	4.855	-4.770	8.997	1.00	41.13	AAAA
	ATOM	1183	NE	ARG	A	164	5.368	-6.140	8.946	1.00	43.44	AAAA
	ATOM	1184	CZ	ARG	A	164	4.765	-7.145	8.311	1.00	44.08	AAAA
	ATOM	1185	NH1	ARG	A	164	3.619	-6.940	7.671	1.00	44.91	AAAA
	ATOM	1186	NH2	ARG	A	164	5.308	-8.355	8.308	1.00	44.44	AAAA
	ATOM	1187	C	ARG	A	164	7.649	-3.248	12.419	1.00	34.72	AAAA
	ATOM	1188	O	ARG	A	164	8.364	-2.769	11.537	1.00	33.63	AAAA
	ATOM	1189	N	THR	A	165	8.138	-3.855	13.496	1.00	34.72	AAAA
	ATOM	1190	CA	THR	A	165	9.567	-3.969	13.730	1.00	34.94	AAAA
	ATOM	1191	CB	THR	A	165	9.839	-4.437	15.177	1.00	35.90	AAAA
	ATOM	1192	OG1	THR	A	165	9.008	-5.563	15.488	1.00	36.96	AAAA
	ATOM	1193	CG2	THR	A	165	9.530	-3.313	16.149	1.00	35.88	AAAA
	ATOM	1194	C	THR	A	165	10.373	-4.814	12.749	1.00	34.61	AAAA
	ATOM	1195	O	THR	A	165	11.577	-4.603	12.608	1.00	34.56	AAAA
	ATOM	1196	N	ASP	A	166	9.739	-5.765	12.068	1.00	34.66	AAAA
	ATOM	1197	CA	ASP	A	166	10.492	-6.558	11.103	1.00	34.85	AAAA
	ATOM	1198	CB	ASP	A	166	9.697	-7.784	10.642	1.00	36.47	AAAA
	ATOM	1199	CG	ASP	A	166	8.341	-7.430	10.089	1.00	37.65	AAAA
	ATOM	1200	OD1	ASP	A	166	7.566	-8.365	9.804	1.00	41.03	AAAA
	ATOM	1201	OD2	ASP	A	166	8.048	-6.227	9.937	1.00	39.97	AAAA
	ATOM	1202	C	ASP	A	166	10.862	-5.667	9.917	1.00	33.70	AAAA
	ATOM	1203	O	ASP	A	166	11.846	-5.925	9.224	1.00	34.04	AAAA
	ATOM	1204	N	VAL	A	167	10.081	-4.610	9.694	1.00	31.98	AAAA
	ATOM	1205	CA	VAL	A	167	10.366	-3.667	8.611	1.00	31.43	AAAA
	ATOM	1206	CB	VAL	A	167	9.096	-2.888	8.170	1.00	31.53	AAAA
	ATOM	1207	CG1	VAL	A	167	9.485	-1.738	7.248	1.00	30.83	AAAA
	ATOM	1208	CG2	VAL	A	167	8.120	-3.825	7.458	1.00	31.61	AAAA
	ATOM	1209	C	VAL	A	167	11.400	-2.657	9.108	1.00	31.23	AAAA
	ATOM	1210	O	VAL	A	167	12.320	-2.268	8.380	1.00	30.04	AAAA
	ATOM	1211	N	LEU	A	168	11.243	-2.238	10.359	1.00	31.72	AAAA
	ATOM	1212	CA	LEU	A	168	12.159	-1.277	10.959	1.00	32.61	AAAA
	ATOM	1213	CB	LEU	A	168	11.714	-0.942	12.387	1.00	33.77	AAAA
	ATOM	1214	CG	LEU	A	168	10.490	-0.040	12.562	1.00	34.46	AAAA
	ATOM	1215	CD1	LEU	A	168	10.141	0.076	14.041	1.00	35.50	AAAA
	ATOM	1216	CD2	LEU	A	168	10.790	1.338	11.974	1.00	34.18	AAAA
	ATOM	1217	C	LEU	A	168	13.594	-1.790	10.986	1.00	32.72	AAAA
	ATOM	1218	O	LEU	A	168	14.538	-1.002	10.923	1.00	32.67	AAAA
	ATOM	1219	N	ALA	A	169	13.752	-3.109	11.076	1.00	33.35	AAAA
	ATOM	1220	CA	ALA	A	169	15.077	-3.725	11.138	1.00	34.36	AAAA
	ATOM	1221	CB	ALA	A	169	14.992	-5.054	11.883	1.00	33.96	AAAA
	ATOM	1222	C	ALA	A	169	15.746	-3.939	9.777	1.00	35.45	AAAA
	ATOM	1223	O	ALA	A	169	16.905	-4.362	9.713	1.00	36.53	AAAA
	ATOM	1224	N	LEU	A	170	15.030	-3.651	8.695	1.00	34.52	AAAA
	ATOM	1225	CA	LEU	A	170	15.590	-3.833	7.358	1.00	34.60	AAAA

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ATOM 1227 CG LEU A 170 13.363 -4.333 6.071 1.00 33.98 AAAA
ATOM 1228 CD1 LEU A 170 12.393 -3.675 5.101 1.00 34.11 AAAA
ATOM 1229 CD2 LEU A 170 13.820 -5.688 5.543 1.00 33.52 AAAA
ATOM 1230 C LEU A 170 16.880 -3.042 7.163 1.00 34.41 AAAA
ATOM 1231 O LEU A 170 17.001 -1.902 7.616 1.00 33.45 AAAA
ATOM 1232 N PRO A 171 17.867 -3.648 6.486 1.00 34.33 AAAA
ATOM 1233 CD PRO A 171 17.877 -5.028 5.971 1.00 34.76 AAAA
ATOM 1234 CA PRO A 171 19.152 -2.988 6.233 1.00 35.17 AAAA
ATOM 1235 CB PRO A 171 19.897 -4.005 5.366 1.00 34.52 AAAA
ATOM 1236 CG PRO A 171 19.361 -5.308 5.844 1.00 34.60 AAAA
ATOM 1237 C PRO A 171 18.938 -1.665 5.503 1.00 35.39 AAAA
ATOM 1238 O PRO A 171 17.933 -1.485 4.820 1.00 34.32 AAAA
ATOM 1239 N LEU A 172 19.884 -0.746 5.654 1.00 36.05 AAAA
ATOM 1240 CA LEU A 172 19.801 0.555 4.998 1.00 37.43 AAAA
ATOM 1241 CB LEU A 172 20.946 1.458 5.468 1.00 37.48 AAAA
ATOM 1242 CG LEU A 172 20.934 1.934 6.925 1.00 38.42 AAAA
ATOM 1243 CD1 LEU A 172 19.751 2.863 7.158 1.00 37.89 AAAA
ATOM 1244 CD2 LEU A 172 20.876 0.735 7.859 1.00 38.70 AAAA
ATOM 1245 C LEU A 172 19.865 0.400 3.479 1.00 38.03 AAAA
ATOM 1246 O LEU A 172 20.392 -0.591 2.969 1.00 38.19 AAAA
ATOM 1247 N PRO A 173 19.329 1.383 2.737 1.00 38.41 AAAA
ATOM 1248 CD PRO A 173 18.647 2.586 3.248 1.00 38.12 AAAA
ATOM 1249 CA PRO A 173 19.319 1.367 1.271 1.00 39.54 AAAA
ATOM 1250 CB PRO A 173 18.853 2.778 0.923 1.00 38.97 AAAA
ATOM 1251 CG PRO A 173 17.898 3.076 2.029 1.00 38.41 AAAA
ATOM 1252 C PRO A 173 20.672 1.027 0.639 1.00 41.06 AAAA
ATOM 1253 O PRO A 173 20.751 0.205 -0.276 1.00 41.26 AAAA
ATOM 1254 N GLN A 174 21.734 1.659 1.127 1.00 42.31 AAAA
ATOM 1255 CA GLN A 174 23.063 1.401 0.591 1.00 43.56 AAAA
ATOM 1256 CB GLN A 174 24.118 2.219 1.343 1.00 45.08 AAAA
ATOM 1257 CG GLN A 174 24.197 3.672 0.906 1.00 47.91 AAAA
ATOM 1258 CD GLN A 174 25.366 4.413 1.534 1.00 50.04 AAAA
ATOM 1259 OE1 GLN A 174 25.665 5.552 1.164 1.00 50.92 AAAA
ATOM 1260 NE2 GLN A 174 26.033 3.771 2.491 1.00 50.23 AAAA
ATOM 1261 C GLN A 174 23.415 -0.076 0.667 1.00 43.25 AAAA
ATOM 1262 O GLN A 174 23.955 -0.641 -0.280 1.00 42.73 AAAA
ATOM 1263 N GLN A 175 23.098 -0.702 1.794 1.00 43.02 AAAA
ATOM 1264 CA GLN A 175 23.398 -2.115 1.981 1.00 43.41 AAAA
ATOM 1265 CB GLN A 175 23.206 -2.505 3.449 1.00 44.88 AAAA
ATOM 1266 CG GLN A 175 23.844 -1.544 4.444 1.00 47.91 AAAA
ATOM 1267 CD GLN A 175 25.331 -1.344 4.211 1.00 49.82 AAAA
ATOM 1268 OE1 GLN A 175 25.747 -0.765 3.203 1.00 50.30 AAAA
ATOM 1269 NE2 GLN A 175 26.145 -1.826 5.148 1.00 51.04 AAAA
ATOM 1270 C GLN A 175 22.521 -2.997 1.097 1.00 42.34 AAAA

	ATOM	1271	O	GLN	A	175	22.996	-3.961	0.500	1.00	41.64	AAAA
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	ATOM	1273	CA	ARG	A	176	20.285	-3.422	0.216	1.00	41.37	AAAA
	ATOM	1274	CB	ARG	A	176	18.854	-2.912	0.469	1.00	42.69	AAAA
5	ATOM	1275	CG	ARG	A	176	17.767	-3.726	-0.232	1.00	44.32	AAAA
	ATOM	1276	CD	ARG	A	176	16.338	-3.227	0.066	1.00	46.28	AAAA
	ATOM	1277	NE	ARG	A	176	15.922	-2.116	-0.793	1.00	46.82	AAAA
	ATOM	1278	CZ	ARG	A	176	16.043	-0.829	-0.479	1.00	47.07	AAAA
	ATOM	1279	NH1	ARG	A	176	16.567	-0.471	0.686	1.00	47.74	AAAA
10	ATOM	1280	NH2	ARG	A	176	15.645	0.102	-1.337	1.00	46.75	AAAA
	ATOM	1281	C	ARG	A	176	20.574	-3.358	-1.279	1.00	40.60	AAAA
	ATOM	1282	O	ARG	A	176	20.485	-4.366	-1.981	1.00	39.33	AAAA
	ATOM	1283	N	LEU	A	177	20.928	-2.171	-1.757	1.00	40.82	AAAA
	ATOM	1284	CA	LEU	A	177	21.182	-1.957	-3.177	1.00	41.69	AAAA
15	ATOM	1285	CB	LEU	A	177	20.635	-0.587	-3.580	1.00	41.42	AAAA
	ATOM	1286	CG	LEU	A	177	19.152	-0.376	-3.262	1.00	41.85	AAAA
	ATOM	1287	CD1	LEU	A	177	18.756	1.059	-3.578	1.00	41.44	AAAA
	ATOM	1288	CD2	LEU	A	177	18.311	-1.358	-4.066	1.00	41.27	AAAA
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	ATOM	1291	N	ALA	A	178	23.536	-2.374	-2.709	1.00	42.36	AAAA
	ATOM	1292	CA	ALA	A	178	24.951	-2.505	-3.047	1.00	41.77	AAAA
	ATOM	1293	CB	ALA	A	178	25.774	-2.711	-1.778	1.00	42.52	AAAA
	ATOM	1294	C	ALA	A	178	25.204	-3.649	-4.024	1.00	41.23	AAAA
25	ATOM	1295	O	ALA	A	178	24.981	-4.818	-3.701	1.00	41.31	AAAA
	ATOM	1296	N	GLY	A	179	25.668	-3.299	-5.221	1.00	40.21	AAAA
	ATOM	1297	CA	GLY	A	179	25.960	-4.298	-6.232	1.00	37.93	AAAA
	ATOM	1298	C	GLY	A	179	24.747	-4.873	-6.938	1.00	36.85	AAAA
	ATOM	1299	O	GLY	A	179	24.873	-5.797	-7.744	1.00	36.55	AAAA
30	ATOM	1300	N	ARG	A	180	23.566	-4.333	-6.654	1.00	35.52	AAAA
	ATOM	1301	CA	ARG	A	180	22.362	-4.844	-7.289	1.00	34.04	AAAA
	ATOM	1302	CB	ARG	A	180	21.114	-4.428	-6.504	1.00	31.99	AAAA
	ATOM	1303	CG	ARG	A	180	19.840	-5.038	-7.055	1.00	29.72	AAAA
	ATOM	1304	CD	ARG	A	180	18.608	-4.609	-6.268	1.00	27.51	AAAA
35	ATOM	1305	NE	ARG	A	180	18.531	-5.233	-4.948	1.00	25.67	AAAA
	ATOM	1306	CZ	ARG	A	180	17.475	-5.139	-4.144	1.00	26.02	AAAA
	ATOM	1307	NH1	ARG	A	180	16.414	-4.441	-4.533	1.00	24.19	AAAA
	ATOM	1308	NH2	ARG	A	180	17.472	-5.749	-2.961	1.00	23.88	AAAA
	ATOM	1309	C	ARG	A	180	22.251	-4.353	-8.726	1.00	34.92	AAAA
40	ATOM	1310	O	ARG	A	180	22.348	-3.157	-8.995	1.00	35.69	AAAA
	ATOM	1311	N	GLU	A	181	22.055	-5.290	-9.646	1.00	34.98	AAAA
	ATOM	1312	CA	GLU	A	181	21.917	-4.969	-11.059	1.00	35.58	AAAA
	ATOM	1313	CB	GLU	A	181	23.188	-5.354	-11.822	1.00	37.16	AAAA
	ATOM	1314	CG	GLU	A	181	24.411	-4.540	-11.436	1.00	40.11	AAAA
45	ATOM	1315	CD	GLU	A	181	25.666	-4.983	-12.169	1.00	42.11	AAAA

	ATOM	1316	OE1	GLU	A	181	26.698	-4.284	-12.056	1.00	42.94	AAAA
	ATOM	1317	OE2	GLU	A	181	25.623	-6.033	-12.848	1.00	43.38	AAAA
	ATOM	1318	C	GLU	A	181	20.736	-5.745	-11.615	1.00	34.83	AAAA
	ATOM	1319	O	GLU	A	181	20.148	-6.577	-10.919	1.00	35.81	AAAA
	ATOM	1320	N	GLY	A	182	20.387	-5.469	-12.866	1.00	33.11	AAAA
	ATOM	1321	CA	GLY	A	182	19.279	-6.166	-13.489	1.00	31.63	AAAA
	ATOM	1322	C	GLY	A	182	17.989	-5.368	-13.523	1.00	30.40	AAAA
	ATOM	1323	O	GLY	A	182	17.959	-4.210	-13.106	1.00	28.65	AAAA
	ATOM	1324	N	PRO	A	183	16.898	-5.974	-14.015	1.00	29.29	AAAA
	ATOM	1325	CD	PRO	A	183	16.829	-7.363	-14.498	1.00	30.43	AAAA
	ATOM	1326	CA	PRO	A	183	15.589	-5.327	-14.109	1.00	29.46	AAAA
	ATOM	1327	CB	PRO	A	183	14.675	-6.463	-14.560	1.00	29.59	AAAA
	ATOM	1328	CG	PRO	A	183	15.597	-7.333	-15.362	1.00	30.17	AAAA
	ATOM	1329	C	PRO	A	183	15.159	-4.734	-12.771	1.00	29.01	AAAA
	ATOM	1330	O	PRO	A	183	15.455	-5.289	-11.708	1.00	27.87	AAAA
	ATOM	1331	N	VAL	A	184	14.483	-3.591	-12.826	1.00	27.36	AAAA
	ATOM	1332	CA	VAL	A	184	14.014	-2.942	-11.613	1.00	25.28	AAAA
	ATOM	1333	CB	VAL	A	184	13.506	-1.512	-11.912	1.00	26.16	AAAA
	ATOM	1334	CG1	VAL	A	184	12.865	-0.901	-10.673	1.00	25.72	AAAA
	ATOM	1335	CG2	VAL	A	184	14.670	-0.648	-12.374	1.00	26.35	AAAA
	ATOM	1336	C	VAL	A	184	12.896	-3.799	-11.032	1.00	23.68	AAAA
	ATOM	1337	O	VAL	A	184	11.971	-4.195	-11.735	1.00	21.69	AAAA
	ATOM	1338	N	ARG	A	185	13.003	-4.102	-9.744	1.00	23.12	AAAA
	ATOM	1339	CA	ARG	A	185	12.015	-4.931	-9.065	1.00	22.35	AAAA
	ATOM	1340	CB	ARG	A	185	12.687	-5.649	-7.897	1.00	23.23	AAAA
	ATOM	1341	CG	ARG	A	185	13.910	-6.440	-8.323	1.00	25.75	AAAA
	ATOM	1342	CD	ARG	A	185	14.729	-6.847	-7.120	1.00	27.07	AAAA
	ATOM	1343	NE	ARG	A	185	15.976	-7.502	-7.495	1.00	28.67	AAAA
	ATOM	1344	CZ	ARG	A	185	16.784	-8.093	-6.623	1.00	29.19	AAAA
	ATOM	1345	NH1	ARG	A	185	16.462	-8.100	-5.339	1.00	26.72	AAAA
	ATOM	1346	NH2	ARG	A	185	17.903	-8.679	-7.032	1.00	31.00	AAAA
	ATOM	1347	C	ARG	A	185	10.860	-4.066	-8.574	1.00	21.55	AAAA
	ATOM	1348	O	ARG	A	185	11.033	-3.228	-7.693	1.00	21.13	AAAA
	ATOM	1349	N	VAL	A	186	9.687	-4.263	-9.166	1.00	21.59	AAAA
	ATOM	1350	CA	VAL	A	186	8.515	-3.480	-8.805	1.00	21.51	AAAA
	ATOM	1351	CB	VAL	A	186	7.745	-3.005	-10.064	1.00	21.61	AAAA
	ATOM	1352	CG1	VAL	A	186	6.574	-2.124	-9.656	1.00	21.27	AAAA
	ATOM	1353	CG2	VAL	A	186	8.689	-2.252	-11.001	1.00	22.25	AAAA
	ATOM	1354	C	VAL	A	186	7.563	-4.294	-7.942	1.00	20.09	AAAA
	ATOM	1355	O	VAL	A	186	7.064	-5.330	-8.361	1.00	20.16	AAAA
	ATOM	1356	N	LEU	A	187	7.325	-3.807	-6.735	1.00	20.75	AAAA
	ATOM	1357	CA	LEU	A	187	6.421	-4.462	-5.801	1.00	21.10	AAAA
	ATOM	1358	CB	LEU	A	187	6.979	-4.363	-4.379	1.00	22.77	AAAA
	ATOM	1359	CG	LEU	A	187	6.492	-5.359	-3.316	1.00	24.90	AAAA
	ATOM	1360	CD1	LEU	A	187	6.763	-4.768	-1.932	1.00	23.74	AAAA

	ATOM	1361	CD2	LEU	A	187	5.027	-5.651	-3.487	1.00	27.67	AAAA
	ATOM	1362	C	LEU	A	187	5.104	-3.691	-5.871	1.00	21.37	AAAA
	ATOM	1363	O	LEU	A	187	5.078	-2.491	-5.585	1.00	21.09	AAAA
	ATOM	1364	N	VAL	A	188	4.034	-4.377	-6.262	1.00	21.43	AAAA
5	ATOM	1365	CA	VAL	A	188	2.706	-3.774	-6.355	1.00	22.58	AAAA
	ATOM	1366	CB	VAL	A	188	1.988	-4.190	-7.657	1.00	22.95	AAAA
	ATOM	1367	CG1	VAL	A	188	0.643	-3.488	-7.765	1.00	22.98	AAAA
	ATOM	1368	CG2	VAL	A	188	2.853	-3.842	-8.855	1.00	23.03	AAAA
	ATOM	1369	C	VAL	A	188	1.891	-4.267	-5.161	1.00	22.98	AAAA
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	ATOM	1371	N	VAL	A	189	1.534	-3.349	-4.267	1.00	23.91	AAAA
	ATOM	1372	CA	VAL	A	189	0.779	-3.706	-3.070	1.00	25.11	AAAA
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	ATOM	1374	CG1	VAL	A	189	0.740	-3.635	-0.549	1.00	23.23	AAAA
15	ATOM	1375	CG2	VAL	A	189	2.915	-3.828	-1.773	1.00	22.20	AAAA
	ATOM	1376	C	VAL	A	189	-0.619	-3.096	-3.080	1.00	26.20	AAAA
	ATOM	1377	O	VAL	A	189	-0.770	-1.879	-3.186	1.00	26.94	AAAA
	ATOM	1378	N	GLY	A	190	-1.629	-3.955	-2.975	1.00	27.50	AAAA
	ATOM	1379	CA	GLY	A	190	-3.007	-3.505	-2.966	1.00	30.27	AAAA
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ATOM 2309 OD2 ASP A 313 -0.610 5.514 -22.896 1.00 48.38 AAAA
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ATOM 2311 O ASP A 313 3.069 6.452 -18.832 1.00 39.95 AAAA
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	ATOM	4108	O	MET	B	202	16.189	-23.929	-5.354	1.00 24.40	BBBB
	ATOM	4109	N	PRO	B	203	14.636	-25.059	-4.192	1.00 24.12	BBBB
5	ATOM	4110	CD	PRO	B	203	13.518	-25.991	-3.970	1.00 22.27	BBBB
	ATOM	4111	CA	PRO	B	203	14.608	-23.963	-3.220	1.00 23.84	BBBB
	ATOM	4112	CB	PRO	B	203	13.553	-24.424	-2.217	1.00 24.46	BBBB
	ATOM	4113	CG	PRO	B	203	12.593	-25.178	-3.084	1.00 24.04	BBBB
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	ATOM	4117	CA	GLN	B	204	18.033	-24.708	-1.684	1.00 26.34	BBBB
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	ATOM	4119	CG	GLN	B	204	17.555	-26.626	-0.065	1.00 33.65	BBBB
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	ATOM	4121	OE1	GLN	B	204	18.991	-28.354	0.792	1.00 39.30	BBBB
	ATOM	4122	NE2	GLN	B	204	16.924	-28.960	0.140	1.00 38.32	BBBB
	ATOM	4123	C	GLN	B	204	19.030	-24.177	-2.717	1.00 25.36	BBBB
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	ATOM	4126	CA	VAL	B	205	19.672	-24.033	-5.043	1.00 24.44	BBBB
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	ATOM	4131	O	VAL	B	205	20.487	-21.789	-5.270	1.00 25.25	BBBB
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	ATOM	4134	CB	ALA	B	206	16.466	-20.377	-4.908	1.00 21.55	BBBB
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	ATOM	4144	CB	LYS	B	208	23.432	-21.989	-3.300	1.00 29.85	BBBB
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	ATOM	4146	CD	LYS	B	208	23.264	-22.667	-0.886	1.00 35.74	BBBB
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	ATOM	4148	NZ	LYS	B	208	21.227	-23.899	-0.135	1.00 35.29	BBBB
	ATOM	4149	C	LYS	B	208	23.237	-19.624	-4.050	1.00 27.83	BBBB
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	ATOM	4166	CG	ASP	B	211	20.351	-10.545	-5.768	1.00	31.43	BBBB
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	ATOM	4168	OD2	ASP	B	211	19.323	-11.025	-5.249	1.00	33.41	BBBB
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	ATOM	4187	OG1	THR	B	214	13.323	-14.273	-11.870	1.00	21.93	BBBB
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	ATOM	4193	CB	ILE	B	215	13.417	-19.828	-10.008	1.00	18.82	BBBB
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5	ATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34	BBBB
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	ATOM	4204	CE2	TRP	B	216	5.705	-19.988	-15.085	1.00	19.98	BBBB
10	ATOM	4205	CE3	TRP	B	216	7.329	-18.690	-16.333	1.00	19.39	BBBB
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	ATOM	4208	CZ2	TRP	B	216	4.713	-19.759	-16.043	1.00	22.06	BBBB
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20	ATOM	4215	CB	HIS	B	217	9.553	-23.419	-9.242	1.00	20.56	BBBB
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45	ATOM	4240	C	GLY	B	220	1.596	-30.110	-9.111	1.00	31.96	BBBB

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ATOM   4285  N   VAL B 227      6.019 -25.738  -2.099  1.00 25.21      BBBB
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	ATOM	5131	CA	SER	B	338	16.008	-30.432	-33.408	1.00 32.41 BBBB
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	ATOM	5138	CB	ILE	B	339	13.989	-33.472	-36.384	1.00 35.51 BBBB
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ATOM   5347  OH2 WAT W  69       4.384 -66.131 -41.203  1.00 34.75      WATR
ATOM   5348  OH2 WAT W  70      20.398  -7.386  -4.280  1.00 30.85      WATR
ATOM   5349  OH2 WAT W  71      -2.444 -70.752 -22.067  1.00 25.46      WATR
ATOM   5350  OH2 WAT W  72      -3.963  -4.914  -5.711  1.00 29.67      WATR
ATOM   5351  OH2 WAT W  73      17.663 -11.040 -34.488  1.00 30.24      WATR
ATOM   5352  OH2 WAT W  74      21.404 -42.041 -26.621  1.00 31.41      WATR
ATOM   5353  OH2 WAT W  75      -1.110 -15.319  -1.089  1.00 31.51      WATR
ATOM   5354  OH2 WAT W  76       0.688  19.730  22.519  1.00 26.71      WATR
ATOM   5355  OH2 WAT W  77      12.113 -69.335 -26.593  1.00 27.11      WATR
ATOM   5356  OH2 WAT W  78      11.725 -25.065 -33.817  1.00 43.79      WATR
ATOM   5357  OH2 WAT W  79     -25.519   9.450  22.092  1.00 28.18      WATR
ATOM   5358  OH2 WAT W  80     -14.673   6.584  16.023  1.00 31.37      WATR
ATOM   5359  OH2 WAT W  81      -2.250  -0.253  -1.741  1.00 29.99      WATR
ATOM   5360  OH2 WAT W  82      -7.300  12.943   8.415  1.00 32.39      WATR
ATOM   5361  OH2 WAT W  83       1.712 -13.629 -13.904  1.00 34.08      WATR
ATOM   5362  OH2 WAT W  84       4.709 -17.478  -6.557  1.00 29.67      WATR
ATOM   5363  OH2 WAT W  85      10.070 -57.496 -44.450  1.00 48.39      WATR
ATOM   5364  OH2 WAT W  86       8.040 -30.281 -10.117  1.00 28.59      WATR
ATOM   5365  OH2 WAT W  87      -1.967 -32.372 -38.643  1.00 31.55      WATR
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ATOM   5366  OH2 WAT W  88     -3.178 -64.576 -25.506  1.00 33.66      WATR
ATOM   5367  OH2 WAT W  89     15.762  -9.860 -10.400  1.00 34.29      WATR
ATOM   5368  OH2 WAT W  90      5.654 -30.990 -27.758  1.00 35.84      WATR
ATOM   5369  OH2 WAT W  91     14.959 -46.096 -42.270  1.00 35.21      WATR
ATOM   5370  OH2 WAT W  92     10.137 -13.308  -9.753  1.00 32.65      WATR
ATOM   5371  OH2 WAT W  93     -4.480   6.624   6.614  1.00 27.37      WATR
ATOM   5372  OH2 WAT W  94    -14.574  22.522  18.870  1.00 49.48      WATR
ATOM   5373  OH2 WAT W  95    -11.031 -42.768 -39.637  1.00 37.63      WATR
ATOM   5374  OH2 WAT W  96      9.906 -35.479 -19.203  1.00 29.59      WATR
ATOM   5375  OH2 WAT W  97     -0.990  -0.781  36.951  1.00 37.27      WATR
ATOM   5376  OH2 WAT W  98    -11.422   9.059  11.252  1.00 30.43      WATR
ATOM   5377  OH2 WAT W  99      8.118 -36.710 -22.371  1.00 34.85      WATR
ATOM   5378  OH2 WAT W 100     12.414 -67.326 -22.791  1.00 31.24      WATR
ATOM   5379  OH2 WAT W 101     28.541 -24.603 -31.049  1.00 40.14      WATR
ATOM   5380  OH2 WAT W 102     16.276 -10.934  -3.673  1.00 33.80      WATR
ATOM   5381  OH2 WAT W 103     30.979 -13.264 -22.953  1.00 24.73      WATR
ATOM   5382  OH2 WAT W 104     12.759 -31.636 -31.838  1.00 26.40      WATR
ATOM   5383  OH2 WAT W 105     23.507 -29.661 -32.187  1.00 29.62      WATR
ATOM   5384  OH2 WAT W 106     21.292 -13.141 -24.874  1.00 37.83      WATR
ATOM   5385  OH2 WAT W 107     10.171 -32.960 -15.580  1.00 26.59      WATR
ATOM   5386  OH2 WAT W 108     -2.207   2.376   2.034  1.00 27.55      WATR
ATOM   5387  OH2 WAT W 109     -6.984  22.588  16.082  1.00 39.01      WATR
ATOM   5388  OH2 WAT W 110     14.308 -11.038 -15.406  1.00 26.48      WATR
ATOM   5389  OH2 WAT W 111     10.612   9.749  24.161  1.00 40.18      WATR
ATOM   5390  OH2 WAT W 112      2.406 -15.823 -10.196  1.00 27.61      WATR
ATOM   5391  OH2 WAT W 113      6.310 -68.984 -20.661  1.00 40.25      WATR
ATOM   5392  OH2 WAT W 114     14.379 -10.930  -8.565  1.00 35.86      WATR
ATOM   5393  OH2 WAT W 115     24.183 -35.475 -30.338  1.00 35.17      WATR
ATOM   5394  OH2 WAT W 116     21.897 -31.717  -1.243  1.00 47.61      WATR
ATOM   5395  OH2 WAT W 117     24.065 -17.545 -13.707  1.00 32.24      WATR
ATOM   5396  OH2 WAT W 118     16.772 -51.926 -25.940  1.00 38.66      WATR
ATOM   5397  OH2 WAT W 119     -5.862   6.629   4.446  1.00 39.57      WATR
ATOM   5398  OH2 WAT W 120     14.133 -57.303 -28.159  1.00 30.19      WATR
ATOM   5399  OH2 WAT W 121    -16.538  -6.724  21.638  1.00 40.50      WATR
ATOM   5400  OH2 WAT W 122     19.669 -18.487 -33.216  1.00 38.38      WATR
ATOM   5401  OH2 WAT W 123     15.481   1.078  -4.048  1.00 32.28      WATR
ATOM   5402  OH2 WAT W 124     20.395 -13.033  -2.072  1.00 49.69      WATR
ATOM   5403  OH2 WAT W 125     15.526  -1.437 -15.842  1.00 36.06      WATR
ATOM   5404  OH2 WAT W 126      7.297 -29.419  -1.509  1.00 34.75      WATR
ATOM   5405  OH2 WAT W 127      9.994 -12.069 -21.013  1.00 32.21      WATR
ATOM   5406  OH2 WAT W 128     17.433 -42.825 -16.713  1.00 31.02      WATR
ATOM   5407  OH2 WAT W 129    -15.855  20.882  21.019  1.00 44.11      WATR
ATOM   5408  OH2 WAT W 130     -6.351  -7.687 -14.067  1.00 35.04      WATR
ATOM   5409  OH2 WAT W 131      7.954 -17.872  -1.475  1.00 28.45      WATR
ATOM   5410  OH2 WAT W 132     13.526 -34.593 -31.844  1.00 31.12      WATR
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ATOM   5411  OH2 WAT W 133       9.992 -41.228 -23.098  1.00 26.45      WATR
ATOM   5412  OH2 WAT W 134       8.434  18.132  16.019  1.00 32.97      WATR
ATOM   5413  OH2 WAT W 135      -1.208 -33.658 -36.216  1.00 38.33      WATR
ATOM   5414  OH2 WAT W 136     -14.502   9.100  12.433  1.00 43.21      WATR
ATOM   5415  OH2 WAT W 137      14.394 -43.675 -17.325  1.00 32.32      WATR
ATOM   5416  OH2 WAT W 138      -4.809 -30.333 -46.416  1.00 42.65      WATR
ATOM   5417  OH2 WAT W 139      18.861 -35.072 -35.671  1.00 43.56      WATR
ATOM   5418  OH2 WAT W 140     -10.162 -60.139 -32.862  1.00 35.41      WATR
ATOM   5419  OH2 WAT W 141       6.740 -32.411 -35.303  1.00 38.57      WATR
ATOM   5420  OH2 WAT W 142     -12.257 -60.854 -39.307  1.00 32.90      WATR
ATOM   5421  OH2 WAT W 143      18.910 -40.984 -13.084  1.00 43.43      WATR
ATOM   5422  OH2 WAT W 144      18.857 -49.375 -28.645  1.00 31.34      WATR
ATOM   5423  OH2 WAT W 145       0.235 -17.424 -16.608  1.00 38.85      WATR
ATOM   5424  OH2 WAT W 146      14.236 -11.252 -24.086  1.00 27.79      WATR
ATOM   5425  OH2 WAT W 147      31.513 -22.336 -22.128  1.00 43.18      WATR
ATOM   5426  OH2 WAT W 148      -5.314 -70.396 -26.090  1.00 43.91      WATR
ATOM   5427  OH2 WAT W 149      -7.717 -64.969 -36.808  1.00 26.30      WATR
ATOM   5428  OH2 WAT W 150      22.584 -12.594  -4.179  1.00 46.91      WATR
ATOM   5429  OH2 WAT W 151     -12.388   9.493  36.619  1.00 32.82      WATR
ATOM   5430  OH2 WAT W 152     -14.517  16.479  37.760  1.00 39.52      WATR
ATOM   5431  OH2 WAT W 153     -10.095 -34.647 -29.068  1.00 41.08      WATR
ATOM   5432  OH2 WAT W 154      -5.233  -4.134  31.160  1.00 35.31      WATR
ATOM   5433  OH2 WAT W 155      -6.322  11.278  -1.883  1.00 35.75      WATR
ATOM   5434  OH2 WAT W 156      10.262  -9.572 -16.736  1.00 42.40      WATR
ATOM   5435  OH2 WAT W 157      22.929 -10.414 -23.566  1.00 36.66      WATR
ATOM   5436  OH2 WAT W 158     -15.987   3.994  16.559  1.00 37.22      WATR
ATOM   5437  OH2 WAT W 159      13.385 -44.923 -46.826  1.00 41.55      WATR
ATOM   5438  OH2 WAT W 160      26.508 -13.616 -18.049  1.00 25.93      WATR
ATOM   5439  OH2 WAT W 161       4.671 -66.907 -17.861  1.00 31.54      WATR
ATOM   5440  OH2 WAT W 162     -12.589  12.262  11.825  1.00 32.71      WATR
ATOM   5441  OH2 WAT W 163      13.899 -62.269 -25.144  1.00 30.71      WATR
ATOM   5442  OH2 WAT W 164     -31.053  15.663  19.272  1.00 30.19      WATR
ATOM   5443  OH2 WAT W 165       9.797 -47.899 -25.140  1.00 26.79      WATR
ATOM   5444  OH2 WAT W 166       0.877 -51.774 -25.619  1.00 30.02      WATR
ATOM   5445  OH2 WAT W 167     -17.088  16.246  37.180  1.00 25.63      WATR
ATOM   5446  OH2 WAT W 168       0.855 -52.086 -22.078  1.00 40.99      WATR
ATOM   5447  OH2 WAT W 169     -14.873  18.295  21.203  1.00 40.28      WATR
ATOM   5448  OH2 WAT W 170      11.913 -62.134 -35.641  1.00 41.33      WATR
ATOM   5449  OH2 WAT W 171      25.783 -23.984 -33.162  1.00 44.03      WATR
ATOM   5450  OH2 WAT W 172       7.169 -50.047 -23.737  1.00 47.85      WATR
ATOM   5451  OH2 WAT W 173      20.074 -42.845 -14.939  1.00 32.87      WATR
ATOM   5452  OH2 WAT W 174       8.765   5.909   9.193  1.00 34.30      WATR
ATOM   5453  OH2 WAT W 175      -4.953 -64.494 -45.351  1.00 47.11      WATR
ATOM   5454  OH2 WAT W 176      11.889 -61.263 -22.531  1.00 36.63      WATR
ATOM   5455  OH2 WAT W 177       2.149 -49.169 -24.836  1.00 39.21      WATR
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ATOM   5456  OH2 WAT W 178     -14.051   6.399  13.353  1.00 39.89      WATR
ATOM   5457  OH2 WAT W 179       8.488 -46.760 -23.118  1.00 45.24      WATR
ATOM   5458  OH2 WAT W 180      -1.152 -23.348 -11.975  1.00 30.36      WATR
ATOM   5459  OH2 WAT W 181      -7.002   3.531   7.051  1.00 44.50      WATR
ATOM   5460  OH2 WAT W 182     -12.320 -54.772 -29.990  1.00 38.61      WATR
ATOM   5461  OH2 WAT W 183       6.790 -54.559 -47.733  1.00 44.05      WATR
ATOM   5462  OH2 WAT W 184      26.305 -38.240 -19.177  1.00 39.53      WATR
ATOM   5463  OH2 WAT W 185      20.402 -58.179 -34.391  1.00 46.11      WATR
ATOM   5464  OH2 WAT W 186       8.061 -31.341 -19.653  1.00 41.37      WATR
ATOM   5465  OH2 WAT W 187      -7.549 -15.619  -5.482  1.00 40.60      WATR
ATOM   5466  OH2 WAT W 188     -31.099  11.941  25.471  1.00 38.80      WATR
ATOM   5467  OH2 WAT W 189      28.566 -25.441 -15.103  1.00 34.75      WATR
ATOM   5468  OH2 WAT W 190      -5.613 -40.109 -50.158  1.00 49.21      WATR
ATOM   5469  OH2 WAT W 191      17.024 -13.428   1.709  1.00 39.93      WATR
ATOM   5470  OH2 WAT W 192     -22.114  10.176  37.673  1.00 32.53      WATR
ATOM   5471  OH2 WAT W 193      10.204 -29.330 -20.066  1.00 27.24      WATR
ATOM   5472  OH2 WAT W 194      27.893 -25.793 -21.862  1.00 38.97      WATR
ATOM   5473  OH2 WAT W 195      -5.582  17.681  32.898  1.00 43.64      WATR
ATOM   5474  OH2 WAT W 196      23.004 -45.224 -27.870  1.00 43.04      WATR
ATOM   5475  OH2 WAT W 197       5.189 -58.857 -25.016  1.00 28.15      WATR
ATOM   5476  OH2 WAT W 198      -7.740 -56.165 -24.052  1.00 35.98      WATR
ATOM   5477  OH2 WAT W 199      -8.156  24.723  26.733  1.00 45.54      WATR
ATOM   5478  OH2 WAT W 200      23.286 -32.333 -33.400  1.00 38.12      WATR
ATOM   5479  OH2 WAT W 201      30.646 -14.180 -20.528  1.00 31.01      WATR
ATOM   5480  OH2 WAT W 202      -8.238  -4.609  29.299  1.00 39.76      WATR
ATOM   5481  OH2 WAT W 203      19.370   0.814  -7.532  1.00 35.83      WATR
ATOM   5482  OH2 WAT W 204       0.885 -27.619  -1.442  1.00 47.04      WATR
ATOM   5483  OH2 WAT W 205      16.084 -56.649 -26.382  1.00 45.97      WATR
ATOM   5484  OH2 WAT W 206      -0.698 -19.360  -9.869  1.00 37.53      WATR
ATOM   5485  OH2 WAT W 207       0.682 -14.985 -15.794  1.00 33.35      WATR
ATOM   5486  OH2 WAT W 208       1.646  17.427  31.991  1.00 40.39      WATR
ATOM   5487  OH2 WAT W 209     -21.611   1.533  20.359  1.00 31.04      WATR
ATOM   5488  OH2 WAT W 210      -5.143 -55.137 -45.825  1.00 30.17      WATR
ATOM   5489  OH2 WAT W 211      -9.645  13.045  37.660  1.00 42.93      WATR
ATOM   5490  OH2 WAT W 212      22.096 -11.242 -30.224  1.00 48.12      WATR
ATOM   5491  OH2 WAT W 213      -5.759   2.610 -15.984  1.00 41.67      WATR
ATOM   5492  OH2 WAT W 214      -4.323   7.731  -7.331  1.00 37.92      WATR
ATOM   5493  OH2 WAT W 215      -5.450   7.197  10.632  1.00 33.99      WATR
ATOM   5494  OH2 WAT W 216       2.330 -32.635 -34.500  1.00 38.85      WATR
ATOM   5495  OH2 WAT W 217     -26.827  16.219  13.451  1.00 38.12      WATR
ATOM   5496  OH2 WAT W 218      10.887 -51.427 -23.191  1.00 39.81      WATR
ATOM   5497  OH2 WAT W 219      -9.020  19.746  -3.698  1.00 46.58      WATR
ATOM   5498  OH2 WAT W 220       9.054   6.622  -0.709  1.00 34.14      WATR
ATOM   5499  OH2 WAT W 221       4.173  -7.985 -23.786  1.00 32.75      WATR
ATOM   5500  OH2 WAT W 222       0.983  16.806   3.910  1.00 40.83      WATR
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ATOM	5501	OH2	WAT	W	223	2.222	-16.848	-6.783	1.00	33.50	WATR
ATOM	5502	OH2	WAT	W	224	13.627	1.072	-15.114	1.00	37.51	WATR
ATOM	5503	OH2	WAT	W	225	12.533	-14.212	-9.007	1.00	38.40	WATR
ATOM	5504	OH2	WAT	W	226	1.404	-7.852	5.396	1.00	38.55	WATR
ATOM	5505	OH2	WAT	W	227	31.159	-24.354	-31.143	1.00	37.67	WATR
ATOM	5506	OH2	WAT	W	228	-13.047	-60.728	-42.282	1.00	42.18	WATR
ATOM	5507	OH2	WAT	W	229	8.956	-37.681	-16.765	1.00	41.45	WATR
ATOM	5508	OH2	WAT	W	230	28.749	-13.637	-16.860	1.00	42.34	WATR
ATOM	5509	OH2	WAT	W	231	-4.461	19.451	8.684	1.00	36.17	WATR
ATOM	5510	OH2	WAT	W	232	-9.785	-66.504	-35.701	1.00	44.07	WATR
ATOM	5511	OH2	WAT	W	233	10.673	-41.619	-20.678	1.00	36.58	WATR
ATOM	5512	OH2	WAT	W	234	-15.694	1.684	32.613	1.00	44.04	WATR
ATOM	5513	OH2	WAT	W	235	3.345	1.229	9.738	1.00	35.70	WATR
ATOM	5514	OH2	WAT	W	236	-6.256	-68.913	-30.401	1.00	36.72	WATR
ATOM	5515	OH2	WAT	W	237	28.344	-21.326	-30.399	1.00	36.45	WATR
ATOM	5516	OH2	WAT	W	238	2.876	-34.368	-17.344	1.00	42.48	WATR
ATOM	5517	OH2	WAT	W	239	15.355	-11.202	2.371	1.00	38.84	WATR
ATOM	5518	OH2	WAT	W	240	27.066	-22.336	-6.437	1.00	37.37	WATR
ATOM	5519	OH2	WAT	W	241	2.222	18.464	26.994	1.00	35.75	WATR
ATOM	5520	OH2	WAT	W	242	15.052	-9.829	-31.019	1.00	44.31	WATR
ATOM	5521	OH2	WAT	W	243	10.351	-67.649	-21.184	1.00	35.79	WATR
ATOM	5522	OH2	WAT	W	244	-13.173	14.269	38.605	1.00	41.50	WATR
ATOM	5523	OH2	WAT	W	245	-7.569	9.658	0.793	1.00	37.62	WATR
ATOM	5524	OH2	WAT	W	246	-2.167	-47.395	-19.605	1.00	45.90	WATR
ATOM	5525	OH2	WAT	W	247	7.166	2.400	15.830	1.00	42.90	WATR
ATOM	5526	OH2	WAT	W	248	-11.231	-10.901	-10.057	1.00	45.28	WATR
ATOM	5527	OH2	WAT	W	249	5.684	-16.094	-26.796	1.00	44.76	WATR
ATOM	5528	OH2	WAT	W	250	-4.745	3.667	-18.932	1.00	46.20	WATR
ATOM	5529	OH2	WAT	W	251	-0.505	-22.136	-9.079	1.00	42.89	WATR
ATOM	5530	OH2	WAT	W	252	16.668	-37.987	-7.767	1.00	35.76	WATR
ATOM	5531	OH2	WAT	W	253	2.454	-18.256	-26.130	1.00	43.33	WATR
ATOM	5532	OH2	WAT	W	254	-8.367	-39.960	-21.638	1.00	43.07	WATR
ATOM	5533	OH2	WAT	W	255	15.642	7.805	9.633	1.00	47.78	WATR
ATOM	5534	OH2	WAT	W	256	13.660	-24.331	1.932	1.00	42.50	WATR
ATOM	5535	OH2	WAT	W	257	11.567	-6.104	-23.359	1.00	37.10	WATR
ATOM	5536	OH2	WAT	W	258	18.941	-16.698	0.528	1.00	40.97	WATR
ATOM	5537	OH2	WAT	W	259	-11.441	-63.514	-39.126	1.00	43.17	WATR
ATOM	5538	OH2	WAT	W	260	28.664	-39.605	-22.853	1.00	42.65	WATR
ATOM	5539	OH2	WAT	W	261	6.795	-6.961	31.114	1.00	38.28	WATR
ATOM	5540	OH2	WAT	W	262	7.077	-14.349	-24.858	1.00	41.00	WATR
ATOM	5541	OH2	WAT	W	263	-2.259	-48.991	-29.099	1.00	34.96	WATR
ATOM	5542	OH2	WAT	W	264	21.812	-44.128	-35.641	1.00	44.51	WATR
ATOM	5543	OH2	WAT	W	265	-27.570	4.389	13.296	1.00	48.63	WATR
ATOM	5544	OH2	WAT	W	266	13.573	-27.185	0.220	1.00	43.56	WATR
ATOM	5545	OH2	WAT	W	267	16.549	8.451	-13.582	1.00	44.84	WATR

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ATOM   5546  OH2 WAT W 268     -9.142   9.107  36.872  1.00 37.66      WATR
ATOM   5547  OH2 WAT W 269      5.648 -11.797 -24.893  1.00 45.79      WATR
ATOM   5548  OH2 WAT W 270      3.619 -14.850 -23.652  1.00 34.09      WATR
ATOM   5549  OH2 WAT W 271     -8.129 -11.098 -16.064  1.00 39.37      WATR
ATOM   5550  OH2 WAT W 272    -17.342   8.563   9.979  1.00 46.38      WATR
ATOM   5551  OH2 WAT W 273      8.798 -36.348 -46.119  1.00 37.71      WATR
ATOM   5552  OH2 WAT W 274      9.190 -10.509 -35.865  1.00 45.80      WATR
ATOM   5553  OH2 WAT W 275     13.545 -13.441   3.898  1.00 42.83      WATR
ATOM   5554  OH2 WAT W 276     -7.844   0.944  -2.560  1.00 46.27      WATR
ATOM   5555  OH2 WAT W 277      0.478 -47.721 -55.170  1.00 46.25      WATR
ATOM   5556  OH2 WAT W 278     24.658 -18.359 -11.005  1.00 36.33      WATR
ATOM   5557  OH2 WAT W 279     -4.675  21.561  12.155  1.00 37.17      WATR
ATOM   5558  OH2 WAT W 280      0.382  20.486   4.930  1.00 41.40      WATR
ATOM   5559  OH2 WAT W 281      5.919  18.010  25.033  1.00 41.72      WATR
ATOM   5560  OH2 WAT W 282     -2.987 -63.751 -22.983  1.00 43.76      WATR
ATOM   5561  OH2 WAT W 283      8.990 -33.134 -17.898  1.00 40.17      WATR
ATOM   5562  OH2 WAT W 284      0.155 -61.872 -48.384  1.00 49.87      WATR
ATOM   5563  OH2 WAT W 285    -10.443 -56.965 -24.681  1.00 48.02      WATR
ATOM   5564  OH2 WAT W 286     18.915 -33.048  -3.930  1.00 37.81      WATR
ATOM   5565  OH2 WAT W 287    -16.181  11.706  12.277  1.00 41.77      WATR
ATOM   5566  OH2 WAT W 288      7.197   7.180  10.953  1.00 46.19      WATR
ATOM   5567  OH2 WAT W 289     31.934 -26.155 -26.053  1.00 38.77      WATR
ATOM   5568  OH2 WAT W 290    -15.232  -0.248  11.315  1.00 40.14      WATR
ATOM   5569  OH2 WAT W 291      9.450 -27.963  -1.396  1.00 41.29      WATR
ATOM   5570  OH2 WAT W 292     -1.800  13.139  -9.983  1.00 41.60      WATR
ATOM   5571  OH2 WAT W 293     -7.766   5.988   9.798  1.00 40.11      WATR
ATOM   5572  OH2 WAT W 294      7.973   4.338  14.321  1.00 39.97      WATR
ATOM   5573  OH2 WAT W 295     23.449 -40.563 -27.347  1.00 40.59      WATR
ATOM   5574  OH2 WAT W 296     -3.537 -28.260 -15.925  1.00 42.10      WATR
ATOM   5575  OH2 WAT W 297     28.052 -32.620 -12.168  1.00 48.03      WATR
ATOM   5576  OH2 WAT W 298     20.655 -43.315 -28.829  1.00 40.17      WATR
ATOM   5577  S   SO4 S   1      1.273 -70.953 -23.009  1.00 22.99      SO4
ATOM   5578  O1  SO4 S   1      1.720 -71.882 -24.053  1.00 21.18      SO4
ATOM   5579  O2  SO4 S   1      0.908 -69.659 -23.626  1.00 22.47      SO4
ATOM   5580  O3  SO4 S   1      2.337 -70.752 -22.018  1.00 23.88      SO4
ATOM   5581  O4  SO4 S   1      0.088 -71.522 -22.328  1.00 22.50      SO4
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END
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TABLE 2 ATOMIC COORDINATES OF E. COLI MURG C-ALPHA BACKBONE ATOMS

	ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00 45.28	BBBB
	ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00 38.63	BBBB
	ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00 30.88	BBBB
	ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00 26.66	BBBB
	ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00 23.16	BBBB
	ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00 24.54	BBBB
	ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00 29.43	BBBB
	ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00 33.82	BBBB
	ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00 36.08	BBBB
	ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00 38.51	BBBB
	ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00 36.57	BBBB
	ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00 33.48	BBBB
	ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00 28.22	BBBB
	ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00 27.77	BBBB
	ATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00 29.00	BBBB
	ATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00 26.12	BBBB
	ATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00 25.07	BBBB
	ATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00 25.32	BBBB
	ATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00 25.94	BBBB
	ATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00 25.70	BBBB
	ATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00 26.15	BBBB
	ATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00 29.32	BBBB
	ATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00 32.38	BBBB
	ATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00 32.00	BBBB
	ATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00 34.91	BBBB
	ATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00 37.55	BBBB
	ATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00 38.24	BBBB
	ATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00 35.75	BBBB
	ATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00 34.58	BBBB
	ATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00 35.40	BBBB
	ATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00 34.16	BBBB
	ATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00 31.56	BBBB
	ATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00 27.41	BBBB
	ATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00 24.71	BBBB
	ATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00 23.47	BBBB
	ATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00 29.84	BBBB
	ATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00 38.81	BBBB
	ATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00 44.47	BBBB
	ATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00 40.44	BBBB
	ATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00 36.33	BBBB

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ATOM   2945  CA  GLU B  47     -5.458 -45.655 -25.029  1.00 31.79      BBBB
ATOM   2954  CA  ALA B  48     -8.821 -47.344 -24.414  1.00 32.58      BBBB
ATOM   2959  CA  ASP B  49    -10.143 -44.065 -23.009  1.00 35.60      BBBB
ATOM   2967  CA  LEU B  50     -8.026 -41.484 -24.840  1.00 33.49      BBBB
ATOM   2975  CA  VAL B  51     -8.299 -42.641 -28.449  1.00 32.68      BBBB
ATOM   2983  CA  PRO B  52    -12.111 -42.601 -28.453  1.00 34.43      BBBB
ATOM   2989  CA  LYS B  53    -11.998 -39.054 -27.064  1.00 36.73      BBBB
ATOM   2998  CA  HIS B  54    -10.116 -38.212 -30.259  1.00 34.62      BBBB
ATOM   3008  CA  GLY B  55    -12.938 -39.481 -32.447  1.00 35.34      BBBB
ATOM   3012  CA  ILE B  56    -10.909 -42.517 -33.514  1.00 33.81      BBBB
ATOM   3020  CA  GLU B  57    -12.228 -46.083 -33.467  1.00 34.16      BBBB
ATOM   3029  CA  ILE B  58    -10.217 -48.658 -31.553  1.00 31.38      BBBB
ATOM   3037  CA  ASP B  59    -10.039 -52.442 -31.720  1.00 31.09      BBBB
ATOM   3045  CA  PHE B  60     -8.809 -54.410 -28.713  1.00 30.32      BBBB
ATOM   3056  CA  ILE B  61     -6.832 -57.616 -28.269  1.00 28.55      BBBB
ATOM   3064  CA  ARG B  62     -5.709 -59.416 -25.133  1.00 30.76      BBBB
ATOM   3075  CA  ILE B  63     -2.036 -59.770 -24.231  1.00 31.38      BBBB
ATOM   3083  CA  SER B  64     -2.356 -60.520 -20.505  1.00 37.51      BBBB
ATOM   3089  CA  GLY B  65      0.679 -62.355 -19.199  1.00 37.13      BBBB
ATOM   3093  CA  LEU B  66      2.591 -61.413 -22.355  1.00 33.17      BBBB
ATOM   3101  CA  ARG B  67      3.671 -57.928 -21.277  1.00 30.90      BBBB
ATOM   3112  CA  GLY B  68      7.380 -57.427 -20.685  1.00 26.79      BBBB
ATOM   3116  CA  LYS B  69      8.238 -60.463 -22.796  1.00 23.93      BBBB
ATOM   3125  CA  GLY B  70     10.755 -60.229 -25.636  1.00 22.26      BBBB
ATOM   3129  CA  ILE B  71     10.357 -62.386 -28.762  1.00 23.55      BBBB
ATOM   3137  CA  LYS B  72     12.038 -65.491 -27.343  1.00 24.92      BBBB
ATOM   3146  CA  ALA B  73      9.839 -65.306 -24.233  1.00 21.18      BBBB
ATOM   3151  CA  LEU B  74      6.745 -64.762 -26.387  1.00 19.36      BBBB
ATOM   3159  CA  ILE B  75      7.434 -67.768 -28.601  1.00 21.18      BBBB
ATOM   3167  CA  ALA B  76      7.996 -69.726 -25.374  1.00 21.72      BBBB
ATOM   3172  CA  ALA B  77      4.289 -69.121 -24.655  1.00 21.07      BBBB
ATOM   3178  CA  PRO B  78      2.772 -70.846 -27.771  1.00 20.95      BBBB
ATOM   3184  CA  LEU B  79     -0.896 -70.728 -26.783  1.00 21.32      BBBB
ATOM   3192  CA  ARG B  80     -0.980 -67.115 -25.637  1.00 21.30      BBBB
ATOM   3203  CA  ILE B  81      1.113 -65.621 -28.421  1.00 19.47      BBBB
ATOM   3211  CA  PHE B  82     -0.875 -67.582 -31.038  1.00 19.15      BBBB
ATOM   3222  CA  ASN B  83     -4.150 -66.332 -29.577  1.00 20.90      BBBB
ATOM   3230  CA  ALA B  84     -3.177 -62.647 -29.484  1.00 19.30      BBBB
ATOM   3235  CA  TRP B  85     -1.820 -63.111 -33.032  1.00 20.56      BBBB
ATOM   3249  CA  ARG B  86     -5.140 -64.660 -34.166  1.00 23.28      BBBB
ATOM   3260  CA  GLN B  87     -7.101 -61.802 -32.567  1.00 24.07      BBBB
ATOM   3269  CA  ALA B  88     -4.996 -59.183 -34.355  1.00 23.78      BBBB
ATOM   3274  CA  ARG B  89     -5.285 -61.111 -37.636  1.00 24.94      BBBB
ATOM   3285  CA  ALA B  90     -9.088 -61.151 -37.383  1.00 26.16      BBBB
ATOM   3290  CA  ILE B  91     -9.108 -57.400 -36.733  1.00 26.97      BBBB
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ATOM   3298  CA  MET B  92      -6.872 -56.693 -39.717  1.00 29.03      BBBB
ATOM   3306  CA  LYS B  93      -8.735 -59.038 -42.050  1.00 33.20      BBBB
ATOM   3315  CA  ALA B  94     -11.943 -57.157 -41.183  1.00 33.62      BBBB
ATOM   3320  CA  TYR B  95     -10.504 -53.620 -41.224  1.00 33.83      BBBB
ATOM   3332  CA  LYS B  96      -8.104 -54.327 -44.122  1.00 33.85      BBBB
ATOM   3342  CA  PRO B  97      -5.490 -51.623 -43.419  1.00 31.82      BBBB
ATOM   3348  CA  ASP B  98      -3.049 -50.685 -46.188  1.00 29.78      BBBB
ATOM   3356  CA  VAL B  99      -0.296 -50.214 -43.660  1.00 26.75      BBBB
ATOM   3363  CA  VAL B 100       0.227 -50.613 -39.936  1.00 23.59      BBBB
ATOM   3370  CA  LEU B 101       2.214 -48.199 -37.797  1.00 21.59      BBBB
ATOM   3378  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23      BBBB
ATOM   3382  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93      BBBB
ATOM   3390  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89      BBBB
ATOM   3394  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54      BBBB
ATOM   3398  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37      BBBB
ATOM   3410  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06      BBBB
ATOM   3417  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67      BBBB
ATOM   3423  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03      BBBB
ATOM   3428  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99      BBBB
ATOM   3434  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60      BBBB
ATOM   3438  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97      BBBB
ATOM   3442  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49      BBBB
ATOM   3450  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70      BBBB
ATOM   3455  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84      BBBB
ATOM   3460  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22      BBBB
ATOM   3474  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61      BBBB
ATOM   3480  CA  LEU B 118      -1.069 -60.957 -43.882  1.00 25.70      BBBB
ATOM   3488  CA  GLY B 119       1.354 -59.174 -46.192  1.00 27.80      BBBB
ATOM   3492  CA  ILE B 120       0.568 -55.744 -44.731  1.00 24.85      BBBB
ATOM   3501  CA  PRO B 121       3.625 -53.477 -44.591  1.00 22.63      BBBB
ATOM   3507  CA  VAL B 122       4.743 -52.594 -41.083  1.00 22.03      BBBB
ATOM   3514  CA  VAL B 123       6.200 -49.184 -40.310  1.00 20.82      BBBB
ATOM   3521  CA  LEU B 124       7.749 -48.485 -36.915  1.00 22.10      BBBB
ATOM   3529  CA  HIS B 125       8.814 -45.413 -34.981  1.00 21.42      BBBB
ATOM   3539  CA  GLU B 126      10.947 -45.452 -31.817  1.00 22.15      BBBB
ATOM   3548  CA  GLN B 127      10.682 -42.270 -29.735  1.00 22.81      BBBB
ATOM   3557  CA  ASN B 128      13.406 -43.097 -27.216  1.00 22.96      BBBB
ATOM   3565  CA  GLY B 129      17.203 -43.019 -27.294  1.00 25.36      BBBB
ATOM   3569  CA  ILE B 130      17.160 -46.716 -26.488  1.00 28.00      BBBB
ATOM   3577  CA  ALA B 131      14.978 -49.139 -28.461  1.00 25.88      BBBB
ATOM   3582  CA  GLY B 132      12.007 -50.532 -26.568  1.00 24.05      BBBB
ATOM   3586  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54      BBBB
ATOM   3594  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22      BBBB
ATOM   3601  CA  ASN B 135      10.407 -52.419 -31.324  1.00 20.50      BBBB
ATOM   3609  CA  LYS B 136      13.886 -53.949 -31.144  1.00 22.79      BBBB
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	ATOM	3618	CA	TRP	B	137	12.753	-57.345	-32.424	1.00	22.06	BBBB
	ATOM	3632	CA	LEU	B	138	9.744	-56.188	-34.431	1.00	23.15	BBBB
	ATOM	3640	CA	ALA	B	139	12.128	-54.092	-36.542	1.00	25.29	BBBB
	ATOM	3645	CA	LYS	B	140	13.279	-57.337	-38.182	1.00	28.05	BBBB
5	ATOM	3654	CA	ILE	B	141	9.963	-57.818	-40.016	1.00	26.09	BBBB
	ATOM	3662	CA	ALA	B	142	9.331	-54.107	-40.498	1.00	25.03	BBBB
	ATOM	3667	CA	THR	B	143	9.262	-52.595	-43.984	1.00	26.10	BBBB
	ATOM	3674	CA	LYS	B	144	10.436	-49.238	-42.618	1.00	24.73	BBBB
	ATOM	3683	CA	VAL	B	145	11.947	-48.311	-39.252	1.00	23.62	BBBB
10	ATOM	3690	CA	MET	B	146	12.338	-44.736	-37.993	1.00	23.15	BBBB
	ATOM	3698	CA	GLN	B	147	13.762	-43.418	-34.712	1.00	25.05	BBBB
	ATOM	3707	CA	ALA	B	148	13.559	-40.032	-33.009	1.00	26.88	BBBB
	ATOM	3712	CA	PHE	B	149	17.239	-39.820	-32.098	1.00	29.39	BBBB
	ATOM	3724	CA	PRO	B	150	20.310	-41.541	-33.535	1.00	31.87	BBBB
15	ATOM	3730	CA	GLY	B	151	21.629	-44.537	-31.595	1.00	32.62	BBBB
	ATOM	3734	CA	ALA	B	152	18.447	-46.476	-30.753	1.00	32.71	BBBB
	ATOM	3739	CA	PHE	B	153	18.925	-48.506	-33.937	1.00	34.83	BBBB
	ATOM	3751	CA	PRO	B	154	22.158	-48.751	-35.993	1.00	38.97	BBBB
	ATOM	3757	CA	ASN	B	155	20.765	-47.568	-39.346	1.00	41.08	BBBB
20	ATOM	3765	CA	ALA	B	156	17.170	-46.407	-38.843	1.00	37.55	BBBB
	ATOM	3770	CA	GLU	B	157	16.367	-43.044	-40.460	1.00	34.40	BBBB
	ATOM	3779	CA	VAL	B	158	16.337	-40.344	-37.764	1.00	31.16	BBBB
	ATOM	3786	CA	VAL	B	159	13.155	-38.265	-37.889	1.00	28.10	BBBB
	ATOM	3793	CA	GLY	B	160	12.724	-36.921	-34.355	1.00	26.93	BBBB
25	ATOM	3797	CA	ASN	B	161	9.456	-36.807	-32.375	1.00	25.27	BBBB
	ATOM	3806	CA	PRO	B	162	6.315	-34.747	-33.004	1.00	26.14	BBBB
	ATOM	3812	CA	VAL	B	163	6.456	-31.379	-31.216	1.00	27.75	BBBB
	ATOM	3819	CA	ARG	B	164	3.667	-28.953	-30.246	1.00	32.36	BBBB
	ATOM	3830	CA	THR	B	165	3.038	-26.307	-32.924	1.00	31.74	BBBB
30	ATOM	3837	CA	ASP	B	166	3.252	-23.404	-30.466	1.00	30.64	BBBB
	ATOM	3845	CA	VAL	B	167	6.746	-24.503	-29.440	1.00	25.91	BBBB
	ATOM	3852	CA	LEU	B	168	7.780	-25.002	-33.075	1.00	28.46	BBBB
	ATOM	3860	CA	ALA	B	169	6.580	-21.455	-33.756	1.00	31.43	BBBB
	ATOM	3865	CA	LEU	B	170	9.002	-19.905	-31.268	1.00	29.60	BBBB
35	ATOM	3874	CA	PRO	B	171	11.611	-17.457	-32.642	1.00	30.11	BBBB
	ATOM	3880	CA	LEU	B	172	15.157	-18.780	-33.062	1.00	28.33	BBBB
	ATOM	3889	CA	PRO	B	173	17.450	-18.550	-29.977	1.00	25.25	BBBB
	ATOM	3895	CA	GLN	B	174	19.526	-15.527	-31.049	1.00	25.46	BBBB
	ATOM	3904	CA	GLN	B	175	16.365	-13.525	-31.718	1.00	28.47	BBBB
40	ATOM	3913	CA	ARG	B	176	14.611	-14.635	-28.525	1.00	29.01	BBBB
	ATOM	3924	CA	LEU	B	177	17.673	-13.970	-26.331	1.00	29.90	BBBB
	ATOM	3932	CA	ALA	B	178	18.766	-10.776	-28.131	1.00	30.78	BBBB
	ATOM	3937	CA	GLY	B	179	19.846	-7.993	-25.784	1.00	30.10	BBBB
	ATOM	3941	CA	ARG	B	180	18.676	-9.965	-22.787	1.00	28.97	BBBB
45	ATOM	3952	CA	GLU	B	181	20.545	-9.027	-19.621	1.00	31.79	BBBB

ATOM	3961	CA	GLY	B	182	19.871	-9.586	-15.943	1.00	27.75	BBBB
ATOM	3966	CA	PRO	B	183	19.450	-12.832	-13.913	1.00	22.93	BBBB
ATOM	3972	CA	VAL	B	184	19.524	-16.146	-15.729	1.00	18.01	BBBB
ATOM	3979	CA	ARG	B	185	15.873	-17.216	-16.011	1.00	17.62	BBBB
ATOM	3990	CA	VAL	B	186	15.508	-20.771	-14.741	1.00	16.47	BBBB
ATOM	3997	CA	LEU	B	187	12.361	-22.710	-15.604	1.00	16.75	BBBB
ATOM	4005	CA	VAL	B	188	11.774	-25.775	-13.381	1.00	18.41	BBBB
ATOM	4012	CA	VAL	B	189	9.298	-28.234	-14.948	1.00	22.11	BBBB
ATOM	4019	CA	GLY	B	190	7.914	-31.188	-12.994	1.00	27.28	BBBB
ATOM	4023	CA	GLY	B	191	4.935	-32.163	-15.115	1.00	31.94	BBBB
ATOM	4027	CA	SER	B	192	1.313	-32.665	-14.064	1.00	35.91	BBBB
ATOM	4033	CA	GLN	B	193	2.292	-34.763	-11.033	1.00	38.53	BBBB
ATOM	4042	CA	GLY	B	194	5.398	-32.711	-10.350	1.00	35.02	BBBB
ATOM	4046	CA	ALA	B	195	8.977	-33.819	-9.709	1.00	33.12	BBBB
ATOM	4051	CA	ARG	B	196	9.538	-34.512	-6.010	1.00	32.63	BBBB
ATOM	4062	CA	ILE	B	197	13.329	-34.168	-6.164	1.00	28.10	BBBB
ATOM	4070	CA	LEU	B	198	13.069	-30.833	-8.003	1.00	26.58	BBBB
ATOM	4078	CA	ASN	B	199	10.497	-29.447	-5.563	1.00	27.07	BBBB
ATOM	4086	CA	GLN	B	200	12.955	-30.326	-2.794	1.00	30.10	BBBB
ATOM	4095	CA	THR	B	201	16.215	-29.345	-4.474	1.00	27.34	BBBB
ATOM	4102	CA	MET	B	202	15.567	-26.048	-6.268	1.00	23.68	BBBB
ATOM	4111	CA	PRO	B	203	14.608	-23.963	-3.220	1.00	23.84	BBBB
ATOM	4117	CA	GLN	B	204	18.033	-24.708	-1.684	1.00	26.34	BBBB
ATOM	4126	CA	VAL	B	205	19.672	-24.033	-5.043	1.00	24.44	BBBB
ATOM	4133	CA	ALA	B	206	17.980	-20.610	-5.013	1.00	22.84	BBBB
ATOM	4138	CA	ALA	B	207	19.442	-19.857	-1.576	1.00	26.65	BBBB
ATOM	4143	CA	LYS	B	208	22.915	-20.595	-2.919	1.00	28.31	BBBB
ATOM	4152	CA	LEU	B	209	22.577	-18.640	-6.171	1.00	25.68	BBBB
ATOM	4160	CA	GLY	B	210	20.675	-15.628	-4.804	1.00	26.56	BBBB
ATOM	4164	CA	ASP	B	211	20.370	-12.647	-7.190	1.00	28.28	BBBB
ATOM	4172	CA	SER	B	212	22.098	-14.474	-10.067	1.00	25.73	BBBB
ATOM	4178	CA	VAL	B	213	18.925	-16.308	-11.116	1.00	20.76	BBBB
ATOM	4185	CA	THR	B	214	15.204	-15.726	-11.337	1.00	19.60	BBBB
ATOM	4192	CA	ILE	B	215	13.076	-18.850	-11.169	1.00	18.75	BBBB
ATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34	BBBB
ATOM	4214	CA	HIS	B	217	9.015	-23.303	-10.680	1.00	21.06	BBBB
ATOM	4224	CA	GLN	B	218	6.149	-25.594	-11.735	1.00	24.30	BBBB
ATOM	4233	CA	SER	B	219	5.463	-27.800	-8.684	1.00	26.73	BBBB
ATOM	4239	CA	GLY	B	220	2.855	-30.242	-9.961	1.00	30.53	BBBB
ATOM	4243	CA	LYS	B	221	-0.657	-30.914	-8.628	1.00	35.12	BBBB
ATOM	4252	CA	GLY	B	222	-1.195	-29.899	-5.011	1.00	35.34	BBBB
ATOM	4256	CA	SER	B	223	2.451	-28.934	-4.418	1.00	33.98	BBBB
ATOM	4262	CA	GLN	B	224	2.187	-25.208	-5.186	1.00	33.71	BBBB
ATOM	4271	CA	GLN	B	225	1.823	-24.239	-1.519	1.00	32.32	BBBB
ATOM	4280	CA	SER	B	226	4.701	-26.309	-0.122	1.00	28.30	BBBB

	ATOM	4286	CA	VAL	B	227	7.214	-25.247	-2.791	1.00	24.28	BBBB
	ATOM	4293	CA	GLU	B	228	6.178	-21.592	-2.387	1.00	27.23	BBBB
	ATOM	4302	CA	GLN	B	229	6.853	-22.046	1.329	1.00	28.38	BBBB
	ATOM	4311	CA	ALA	B	230	10.185	-23.754	0.682	1.00	26.18	BBBB
	ATOM	4316	CA	TYR	B	231	11.371	-20.766	-1.366	1.00	25.47	BBBB
	ATOM	4328	CA	ALA	B	232	10.342	-18.322	1.368	1.00	27.51	BBBB
	ATOM	4333	CA	GLU	B	233	12.145	-20.441	3.966	1.00	30.87	BBBB
	ATOM	4342	CA	ALA	B	234	15.215	-20.417	1.714	1.00	28.48	BBBB
	ATOM	4347	CA	GLY	B	235	15.033	-16.627	1.815	1.00	26.23	BBBB
	ATOM	4351	CA	GLN	B	236	14.121	-16.198	-1.870	1.00	25.53	BBBB
	ATOM	4361	CA	PRO	B	237	10.336	-15.587	-1.720	1.00	24.65	BBBB
	ATOM	4367	CA	GLN	B	238	10.277	-13.558	-4.945	1.00	24.29	BBBB
	ATOM	4376	CA	HIS	B	239	10.526	-16.608	-7.201	1.00	22.08	BBBB
	ATOM	4386	CA	LYS	B	240	7.375	-17.589	-9.105	1.00	23.26	BBBB
	ATOM	4395	CA	VAL	B	241	5.740	-20.911	-8.277	1.00	23.78	BBBB
	ATOM	4402	CA	THR	B	242	2.758	-22.301	-10.177	1.00	25.93	BBBB
	ATOM	4409	CA	GLU	B	243	0.999	-25.651	-9.837	1.00	27.03	BBBB
	ATOM	4418	CA	PHE	B	244	0.964	-26.068	-13.620	1.00	26.54	BBBB
	ATOM	4429	CA	ILE	B	245	1.932	-24.242	-16.802	1.00	28.48	BBBB
	ATOM	4437	CA	ASP	B	246	-0.754	-24.396	-19.457	1.00	36.00	BBBB
	ATOM	4445	CA	ASP	B	247	1.245	-22.392	-21.999	1.00	30.74	BBBB
	ATOM	4453	CA	MET	B	248	4.625	-24.136	-22.138	1.00	28.41	BBBB
	ATOM	4461	CA	ALA	B	249	5.512	-22.216	-25.290	1.00	24.67	BBBB
	ATOM	4466	CA	ALA	B	250	5.188	-18.933	-23.390	1.00	21.78	BBBB
	ATOM	4471	CA	ALA	B	251	7.301	-20.259	-20.501	1.00	20.85	BBBB
	ATOM	4476	CA	TYR	B	252	9.972	-21.616	-22.886	1.00	22.78	BBBB
	ATOM	4488	CA	ALA	B	253	10.131	-18.224	-24.636	1.00	23.54	BBBB
	ATOM	4493	CA	TRP	B	254	10.829	-16.534	-21.303	1.00	19.76	BBBB
	ATOM	4507	CA	ALA	B	255	13.399	-19.025	-20.003	1.00	19.51	BBBB
	ATOM	4512	CA	ASP	B	256	17.176	-19.026	-20.434	1.00	17.58	BBBB
	ATOM	4520	CA	VAL	B	257	17.535	-22.603	-19.194	1.00	18.53	BBBB
	ATOM	4527	CA	VAL	B	258	15.208	-25.456	-18.234	1.00	19.32	BBBB
	ATOM	4534	CA	VAL	B	259	15.581	-27.957	-15.374	1.00	19.85	BBBB
	ATOM	4541	CA	CYS	B	260	13.454	-31.055	-15.946	1.00	22.00	BBBB
	ATOM	4547	CA	ARG	B	261	13.170	-34.800	-16.515	1.00	23.75	BBBB
	ATOM	4558	CA	SER	B	262	13.975	-36.189	-19.948	1.00	23.18	BBBB
	ATOM	4564	CA	GLY	B	263	11.026	-38.079	-21.361	1.00	22.85	BBBB
	ATOM	4568	CA	ALA	B	264	11.482	-38.564	-25.115	1.00	24.25	BBBB
	ATOM	4573	CA	LEU	B	265	8.846	-36.037	-26.205	1.00	24.66	BBBB
	ATOM	4581	CA	THR	B	266	10.194	-33.557	-23.657	1.00	22.34	BBBB
	ATOM	4588	CA	VAL	B	267	13.730	-33.762	-25.023	1.00	21.11	BBBB
	ATOM	4595	CA	SER	B	268	12.411	-33.191	-28.567	1.00	21.96	BBBB
	ATOM	4601	CA	GLU	B	269	10.282	-30.272	-27.378	1.00	21.95	BBBB
	ATOM	4610	CA	ILE	B	270	13.295	-28.698	-25.638	1.00	20.62	BBBB
	ATOM	4618	CA	ALA	B	271	15.440	-29.058	-28.776	1.00	22.45	BBBB

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ATOM   4623  CA  ALA B 272      12.719 -27.451 -30.898  1.00 22.17      BBBB
ATOM   4628  CA  ALA B 273      12.361 -24.596 -28.407  1.00 21.97      BBBB
ATOM   4633  CA  GLY B 274      16.093 -24.023 -28.709  1.00 21.07      BBBB
ATOM   4637  CA  LEU B 275      16.666 -24.057 -24.966  1.00 19.78      BBBB
ATOM   4646  CA  PRO B 276      19.651 -25.199 -22.875  1.00 16.62      BBBB
ATOM   4652  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80      BBBB
ATOM   4657  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48      BBBB
ATOM   4665  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59      BBBB
ATOM   4676  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67      BBBB
ATOM   4684  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05      BBBB
ATOM   4690  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13      BBBB
ATOM   4701  CA  GLN B 283      16.319 -43.395 -12.591  1.00 41.11      BBBB
ATOM   4710  CA  HIS B 284      15.641 -46.917 -13.843  1.00 43.69      BBBB
ATOM   4720  CA  LYS B 285      17.767 -49.993 -14.571  1.00 45.34      BBBB
ATOM   4729  CA  ASP B 286      16.949 -49.299 -18.222  1.00 43.26      BBBB
ATOM   4737  CA  ARG B 287      17.951 -45.623 -17.883  1.00 36.28      BBBB
ATOM   4748  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77      BBBB
ATOM   4757  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46      BBBB
ATOM   4766  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55      BBBB
ATOM   4778  CA  TRP B 291      19.542 -42.282 -23.116  1.00 28.07      BBBB
ATOM   4792  CA  ASN B 292      16.902 -39.784 -24.270  1.00 26.06      BBBB
ATOM   4800  CA  ALA B 293      18.926 -36.822 -22.979  1.00 25.69      BBBB
ATOM   4805  CA  LEU B 294      22.354 -38.088 -24.032  1.00 25.90      BBBB
ATOM   4814  CA  PRO B 295      21.998 -36.870 -27.635  1.00 26.15      BBBB
ATOM   4820  CA  LEU B 296      21.521 -33.265 -26.481  1.00 25.42      BBBB
ATOM   4828  CA  GLU B 297      24.354 -33.530 -23.953  1.00 28.78      BBBB
ATOM   4837  CA  LYS B 298      26.644 -34.947 -26.648  1.00 31.90      BBBB
ATOM   4846  CA  ALA B 299      25.773 -31.965 -28.847  1.00 30.38      BBBB
ATOM   4851  CA  GLY B 300      26.777 -29.635 -26.017  1.00 26.18      BBBB
ATOM   4855  CA  ALA B 301      23.214 -28.333 -25.638  1.00 22.50      BBBB
ATOM   4860  CA  ALA B 302      22.516 -29.770 -22.186  1.00 21.78      BBBB
ATOM   4865  CA  LYS B 303      23.979 -31.340 -19.048  1.00 25.86      BBBB
ATOM   4874  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17      BBBB
ATOM   4882  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01      BBBB
ATOM   4890  CA  GLU B 306      21.664 -38.702 -13.061  1.00 34.65      BBBB
ATOM   4899  CA  GLN B 307      20.377 -39.599  -9.613  1.00 40.54      BBBB
ATOM   4909  CA  PRO B 308      23.828 -40.891  -8.484  1.00 43.20      BBBB
ATOM   4915  CA  GLN B 309      25.247 -37.361  -8.787  1.00 43.46      BBBB
ATOM   4924  CA  LEU B 310      22.232 -35.166  -8.022  1.00 39.65      BBBB
ATOM   4932  CA  SER B 311      22.660 -32.714  -5.154  1.00 34.90      BBBB
ATOM   4938  CA  VAL B 312      21.990 -29.074  -4.341  1.00 31.50      BBBB
ATOM   4945  CA  ASP B 313      25.642 -28.202  -4.957  1.00 29.61      BBBB
ATOM   4953  CA  ALA B 314      25.782 -30.099  -8.254  1.00 26.47      BBBB
ATOM   4958  CA  VAL B 315      22.755 -28.215  -9.612  1.00 25.33      BBBB
ATOM   4965  CA  ALA B 316      23.888 -24.872  -8.199  1.00 27.13      BBBB
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ATOM   4970  CA  ASN B 317      27.444 -25.246  -9.518  1.00 28.52      BBBB
ATOM   4978  CA  THR B 318      26.174 -26.371 -12.906  1.00 27.04      BBBB
ATOM   4985  CA  LEU B 319      23.883 -23.370 -13.357  1.00 25.21      BBBB
ATOM   4993  CA  ALA B 320      26.445 -20.931 -11.957  1.00 24.59      BBBB
ATOM   4998  CA  GLY B 321      28.934 -22.031 -14.591  1.00 24.34      BBBB
ATOM   5002  CA  TRP B 322      26.738 -21.007 -17.521  1.00 21.72      BBBB
ATOM   5016  CA  SER B 323      27.141 -17.404 -18.692  1.00 19.04      BBBB
ATOM   5022  CA  ARG B 324      24.725 -15.741 -21.112  1.00 18.09      BBBB
ATOM   5033  CA  GLU B 325      27.220 -16.368 -23.954  1.00 16.96      BBBB
ATOM   5042  CA  THR B 326      27.460 -20.055 -23.070  1.00 16.39      BBBB
ATOM   5049  CA  LEU B 327      23.659 -20.305 -22.780  1.00 17.27      BBBB
ATOM   5057  CA  LEU B 328      23.175 -18.745 -26.222  1.00 17.39      BBBB
ATOM   5065  CA  THR B 329      25.567 -21.335 -27.688  1.00 21.30      BBBB
ATOM   5072  CA  MET B 330      23.771 -24.153 -25.870  1.00 19.91      BBBB
ATOM   5080  CA  ALA B 331      20.412 -22.871 -27.098  1.00 18.49      BBBB
ATOM   5085  CA  GLU B 332      21.626 -22.827 -30.704  1.00 21.47      BBBB
ATOM   5094  CA  ARG B 333      23.040 -26.330 -30.408  1.00 23.77      BBBB
ATOM   5105  CA  ALA B 334      19.648 -27.420 -29.063  1.00 22.88      BBBB
ATOM   5110  CA  ARG B 335      17.795 -25.892 -32.002  1.00 23.54      BBBB
ATOM   5121  CA  ALA B 336      20.330 -27.477 -34.372  1.00 26.85      BBBB
ATOM   5126  CA  ALA B 337      19.740 -30.925 -32.865  1.00 30.89      BBBB
ATOM   5131  CA  SER B 338      16.008 -30.432 -33.408  1.00 32.41      BBBB
ATOM   5137  CA  ILE B 339      13.882 -31.941 -36.187  1.00 34.35      BBBB
ATOM   5146  CA  PRO B 340      10.733 -29.730 -36.600  1.00 34.94      BBBB
ATOM   5152  CA  ASP B 341       8.711 -31.820 -39.056  1.00 33.33      BBBB
ATOM   5160  CA  ALA B 342       8.875 -35.238 -37.411  1.00 29.09      BBBB
ATOM   5165  CA  THR B 343       5.115 -35.696 -37.744  1.00 28.55      BBBB
ATOM   5172  CA  GLU B 344       5.085 -34.933 -41.480  1.00 32.00      BBBB
ATOM   5181  CA  ARG B 345       8.138 -37.123 -42.067  1.00 31.44      BBBB
ATOM   5192  CA  VAL B 346       6.578 -40.151 -40.384  1.00 28.61      BBBB
ATOM   5199  CA  ALA B 347       3.249 -39.617 -42.137  1.00 28.96      BBBB
ATOM   5204  CA  ASN B 348       5.035 -39.286 -45.493  1.00 34.56      BBBB
ATOM   5212  CA  GLU B 349       6.954 -42.540 -44.956  1.00 34.86      BBBB
ATOM   5221  CA  VAL B 350       3.767 -44.306 -43.919  1.00 33.79      BBBB
ATOM   5228  CA  SER B 351       2.196 -42.946 -47.095  1.00 36.67      BBBB
ATOM   5234  CA  ARG B 352       5.114 -44.088 -49.251  1.00 40.03      BBBB
ATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78      BBBB
ATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24      BBBB
ATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71      BBBB
ATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93      BBBB
ATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81      BBBB
END
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TABLE 3 ATOMIC COORDINATES OF E. COLI C-ALPHA BACKBONE AND CONSERVED AMINO ACID RESIDUES

ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00 45.28	BBBB
ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00 38.63	BBBB
ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00 30.88	BBBB
ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00 26.66	BBBB
ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00 23.16	BBBB
ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00 24.54	BBBB
ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00 29.43	BBBB
ATOM	2697	N	GLY	B	14	0.150	-47.934	-27.405	1.00 32.46	BBBB
ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00 33.82	BBBB
ATOM	2699	C	GLY	B	14	-0.107	-46.595	-25.299	1.00 34.82	BBBB
ATOM	2700	O	GLY	B	14	0.975	-46.040	-25.479	1.00 35.47	BBBB
ATOM	2701	N	GLY	B	15	-0.986	-46.188	-24.385	1.00 35.56	BBBB
ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00 36.08	BBBB
ATOM	2703	C	GLY	B	15	0.539	-45.254	-22.683	1.00 36.84	BBBB
ATOM	2704	O	GLY	B	15	1.293	-44.311	-22.426	1.00 36.03	BBBB
ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00 38.51	BBBB
ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00 36.57	BBBB
ATOM	2716	N	GLY	B	18	3.949	-43.752	-23.150	1.00 33.83	BBBB
ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00 33.48	BBBB
ATOM	2718	C	GLY	B	18	3.825	-42.593	-25.378	1.00 33.12	BBBB
ATOM	2719	O	GLY	B	18	4.345	-41.650	-25.984	1.00 35.38	BBBB
ATOM	2720	N	HIS	B	19	3.416	-43.699	-25.988	1.00 30.26	BBBB
ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00 28.22	BBBB
ATOM	2722	CB	HIS	B	19	3.772	-45.349	-27.779	1.00 25.81	BBBB
ATOM	2723	CG	HIS	B	19	4.957	-45.966	-27.094	1.00 25.35	BBBB
ATOM	2724	CD2	HIS	B	19	6.281	-45.694	-27.184	1.00 24.18	BBBB
ATOM	2725	ND1	HIS	B	19	4.845	-47.025	-26.217	1.00 24.57	BBBB
ATOM	2726	CE1	HIS	B	19	6.046	-47.380	-25.798	1.00 23.08	BBBB
ATOM	2727	NE2	HIS	B	19	6.936	-46.589	-26.369	1.00 25.51	BBBB
ATOM	2728	C	HIS	B	19	2.280	-43.370	-28.144	1.00 27.91	BBBB
ATOM	2729	O	HIS	B	19	2.300	-43.049	-29.337	1.00 26.91	BBBB
ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00 27.77	BBBB
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ATOM   4095  CA  THR B 201      16.215 -29.345  -4.474  1.00 27.34      BBBB
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ATOM   4185  CA  THR B 214      15.204 -15.726 -11.337  1.00 19.60      BBBB
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ATOM 4710 CA HIS B 284 15.641 -46.917 -13.843 1.00 43.69 BBBB
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ATOM 4729 CA ASP B 286 16.949 -49.299 -18.222 1.00 43.26 BBBB
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ATOM 4798 O ASN B 292 17.566 -37.687 -25.244 1.00 26.18 BBBB
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ATOM   5252  CA  ALA B 354      1.336 -47.957 -48.212  1.00 47.24      BBBB
ATOM   5257  CA  ARG B 355      2.035 -46.964 -51.824  1.00 52.71      BBBB
ATOM   5268  CA  ALA B 356      4.453 -49.913 -51.809  1.00 54.93      BBBB
ATOM   5273  CA  LEU B 357      7.023 -47.522 -53.289  1.00 57.81      BBBB
END
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TABLE 4 ATOMIC COORDINATES OF THE
DONOR NUCLEOTIDE BINDING SITE

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REMARK   4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   LEU B 187      13.695 -22.128 -15.588  1.00 15.92           N
ATOM      2  CA  LEU B 187      12.361 -22.710 -15.604  1.00 16.75           C
ATOM      3  C   LEU B 187      12.450 -24.146 -15.085  1.00 16.85           C
ATOM      4  O   LEU B 187      13.115 -24.982 -15.688  1.00 17.18           O
ATOM      5  CB  LEU B 187      11.813 -22.701 -17.035  1.00 16.85           C
ATOM      6  CG  LEU B 187      10.445 -23.340 -17.276  1.00 18.63           C
ATOM      7  CD1 LEU B 187       9.368 -22.478 -16.625  1.00 19.42           C
ATOM      8  CD2 LEU B 187      10.198 -23.449 -18.783  1.00 19.11           C
ATOM      9  N   VAL B 188      11.788 -24.426 -13.964  1.00 18.20           N
ATOM     10  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41           C
ATOM     11  C   VAL B 188      10.434 -26.440 -13.739  1.00 19.88           C
ATOM     12  O   VAL B 188       9.371 -25.967 -13.336  1.00 20.39           O
ATOM     13  CB  VAL B 188      11.902 -25.714 -11.842  1.00 18.98           C
ATOM     14  CG1 VAL B 188      12.088 -27.126 -11.270  1.00 18.50           C
ATOM     15  CG2 VAL B 188      13.061 -24.818 -11.449  1.00 18.83           C
ATOM     16  N   VAL B 189      10.493 -27.532 -14.496  1.00 21.55           N
ATOM     17  CA  VAL B 189       9.298 -28.234 -14.948  1.00 22.11           C
ATOM     18  C   VAL B 189       9.191 -29.639 -14.351  1.00 23.90           C
ATOM     19  O   VAL B 189      10.067 -30.478 -14.559  1.00 23.61           O
ATOM     20  CB  VAL B 189       9.299 -28.342 -16.488  1.00 22.50           C
ATOM     21  CG1 VAL B 189       8.009 -29.013 -16.981  1.00 22.70           C
ATOM     22  CG2 VAL B 189       9.470 -26.943 -17.101  1.00 21.26           C
ATOM     23  N   GLY B 190       8.111 -29.887 -13.615  1.00 25.60           N
ATOM     24  CA  GLY B 190       7.914 -31.188 -12.994  1.00 27.28           C
ATOM     25  C   GLY B 190       6.808 -32.026 -13.604  1.00 29.67           C
ATOM     26  O   GLY B 190       6.668 -33.208 -13.283  1.00 29.86           O
ATOM     27  N   GLY B 191       6.025 -31.430 -14.497  1.00 30.56           N
ATOM     28  CA  GLY B 191       4.935 -32.163 -15.115  1.00 31.94           C
ATOM     29  C   GLY B 191       3.676 -32.104 -14.269  1.00 33.11           C
ATOM     30  O   GLY B 191       3.691 -31.556 -13.165  1.00 32.14           O
ATOM     31  N   ALA B 195       7.761 -33.045  -9.938  1.00 33.54           N
ATOM     32  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12           C
ATOM     33  C   ALA B 195       9.423 -33.590  -8.267  1.00 32.87           C
ATOM     34  O   ALA B 195       9.955 -32.533  -7.923  1.00 31.47           O
ATOM     35  CB  ALA B 195      10.073 -33.387 -10.679  1.00 33.17           C
ATOM     36  N   LEU B 198      12.897 -32.223  -7.590  1.00 27.07           N
ATOM     37  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58           C
ATOM     38  C   LEU B 198      12.388 -29.893  -7.006  1.00 26.41           C
ATOM     39  O   LEU B 198      12.930 -28.835  -6.667  1.00 26.35           O
ATOM     40  CB  LEU B 198      12.504 -30.616  -9.412  1.00 25.88           C
ATOM     41  CG  LEU B 198      13.196 -31.408 -10.524  1.00 25.40           C
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	ATOM	42	CD1	LEU	B	198	12.625	-31.007	-11.874	1.00 26.54	C
	ATOM	43	CD2	LEU	B	198	14.692	-31.146	-10.493	1.00 25.94	C
	ATOM	44	N	TYR	B	252	8.723	-21.314	-22.184	1.00 21.27	N
	ATOM	45	CA	TYR	B	252	9.972	-21.616	-22.886	1.00 22.78	C
5	ATOM	46	C	TYR	B	252	10.566	-20.354	-23.516	1.00 23.57	C
	ATOM	47	O	TYR	B	252	11.784	-20.180	-23.550	1.00 23.91	O
	ATOM	48	CB	TYR	B	252	9.726	-22.661	-23.980	1.00 21.62	C
	ATOM	49	CG	TYR	B	252	9.662	-24.100	-23.505	1.00 23.34	C
	ATOM	50	CD1	TYR	B	252	9.003	-25.065	-24.261	1.00 22.88	C
10	ATOM	51	CD2	TYR	B	252	10.288	-24.505	-22.319	1.00 22.30	C
	ATOM	52	CE1	TYR	B	252	8.961	-26.392	-23.861	1.00 24.81	C
	ATOM	53	CE2	TYR	B	252	10.253	-25.838	-21.912	1.00 23.56	C
	ATOM	54	CZ	TYR	B	252	9.590	-26.772	-22.687	1.00 24.26	C
	ATOM	55	OH	TYR	B	252	9.554	-28.088	-22.305	1.00 25.57	O
15	ATOM	56	N	VAL	B	258	16.263	-24.643	-18.818	1.00 18.74	N
	ATOM	57	CA	VAL	B	258	15.208	-25.456	-18.234	1.00 19.32	C
	ATOM	58	C	VAL	B	258	15.799	-26.585	-17.389	1.00 19.70	C
	ATOM	59	O	VAL	B	258	16.808	-27.175	-17.758	1.00 18.96	O
	ATOM	60	CB	VAL	B	258	14.328	-26.100	-19.337	1.00 19.89	C
20	ATOM	61	CG1	VAL	B	258	13.101	-26.754	-18.714	1.00 19.81	C
	ATOM	62	CG2	VAL	B	258	13.907	-25.041	-20.364	1.00 21.59	C
	ATOM	63	N	VAL	B	259	15.167	-26.861	-16.253	1.00 20.24	N
	ATOM	64	CA	VAL	B	259	15.581	-27.957	-15.374	1.00 19.85	C
	ATOM	65	C	VAL	B	259	14.382	-28.890	-15.371	1.00 20.02	C
25	ATOM	66	O	VAL	B	259	13.301	-28.500	-14.942	1.00 21.88	O
	ATOM	67	CB	VAL	B	259	15.850	-27.483	-13.936	1.00 20.08	C
	ATOM	68	CG1	VAL	B	259	16.222	-28.689	-13.059	1.00 20.22	C
	ATOM	69	CG2	VAL	B	259	16.966	-26.453	-13.930	1.00 17.86	C
	ATOM	70	N	CYS	B	260	14.562	-30.111	-15.867	1.00 21.70	N
30	ATOM	71	CA	CYS	B	260	13.454	-31.055	-15.946	1.00 22.00	C
	ATOM	72	C	CYS	B	260	13.903	-32.478	-16.242	1.00 21.86	C
	ATOM	73	O	CYS	B	260	15.087	-32.730	-16.496	1.00 21.34	O
	ATOM	74	CB	CYS	B	260	12.494	-30.618	-17.057	1.00 22.77	C
	ATOM	75	SG	CYS	B	260	13.297	-30.506	-18.711	1.00 22.15	S
35	ATOM	76	N	ARG	B	261	12.937	-33.397	-16.212	1.00 22.34	N
	ATOM	77	CA	ARG	B	261	13.170	-34.800	-16.515	1.00 23.75	C
	ATOM	78	C	ARG	B	261	13.351	-34.871	-18.032	1.00 23.98	C
	ATOM	79	O	ARG	B	261	13.117	-33.883	-18.746	1.00 22.44	O
	ATOM	80	CB	ARG	B	261	11.964	-35.663	-16.104	1.00 27.16	C
40	ATOM	81	CG	ARG	B	261	11.376	-35.337	-14.738	1.00 31.82	C
	ATOM	82	CD	ARG	B	261	11.490	-36.473	-13.732	1.00 36.33	C
	ATOM	83	NE	ARG	B	261	12.865	-36.721	-13.323	1.00 38.48	N
	ATOM	84	CZ	ARG	B	261	13.218	-37.176	-12.125	1.00 37.25	C
	ATOM	85	NH1	ARG	B	261	12.295	-37.433	-11.204	1.00 38.46	N
45	ATOM	86	NH2	ARG	B	261	14.499	-37.370	-11.848	1.00 36.79	N

	ATOM	87	N	SER	B	262	13.740	-36.038	-18.527	1.00 22.00	N
	ATOM	88	CA	SER	B	262	13.975	-36.189	-19.948	1.00 23.18	C
	ATOM	89	C	SER	B	262	13.173	-37.263	-20.676	1.00 22.90	C
	ATOM	90	O	SER	B	262	13.738	-38.179	-21.274	1.00 23.25	O
	ATOM	91	CB	SER	B	262	15.481	-36.377	-20.203	1.00 24.45	C
	ATOM	92	OG	SER	B	262	16.043	-37.326	-19.311	1.00 25.79	O
	ATOM	93	N	GLY	B	263	11.850	-37.151	-20.619	1.00 22.74	N
	ATOM	94	CA	GLY	B	263	11.026	-38.079	-21.361	1.00 22.85	C
	ATOM	95	C	GLY	B	263	11.392	-37.793	-22.813	1.00 24.06	C
	ATOM	96	O	GLY	B	263	11.908	-36.705	-23.121	1.00 22.75	O
	ATOM	97	N	ALA	B	264	11.130	-38.739	-23.708	1.00 23.37	N
	ATOM	98	CA	ALA	B	264	11.482	-38.564	-25.115	1.00 24.25	C
	ATOM	99	C	ALA	B	264	10.843	-37.343	-25.783	1.00 24.29	C
	ATOM	100	O	ALA	B	264	11.523	-36.572	-26.470	1.00 24.33	O
	ATOM	101	CB	ALA	B	264	11.133	-39.829	-25.894	1.00 24.58	C
	ATOM	102	N	LEU	B	265	9.541	-37.167	-25.596	1.00 24.44	N
	ATOM	103	CA	LEU	B	265	8.846	-36.037	-26.205	1.00 24.66	C
	ATOM	104	C	LEU	B	265	9.331	-34.717	-25.613	1.00 24.47	C
	ATOM	105	O	LEU	B	265	9.374	-33.693	-26.301	1.00 23.85	O
	ATOM	106	CB	LEU	B	265	7.332	-36.183	-26.011	1.00 25.33	C
	ATOM	107	CG	LEU	B	265	6.760	-37.544	-26.426	1.00 27.97	C
	ATOM	108	CD1	LEU	B	265	5.242	-37.541	-26.258	1.00 28.21	C
	ATOM	109	CD2	LEU	B	265	7.146	-37.856	-27.878	1.00 27.40	C
	ATOM	110	N	THR	B	266	9.702	-34.747	-24.338	1.00 22.12	N
	ATOM	111	CA	THR	B	266	10.194	-33.557	-23.657	1.00 22.34	C
	ATOM	112	C	THR	B	266	11.535	-33.117	-24.226	1.00 21.15	C
	ATOM	113	O	THR	B	266	11.761	-31.926	-24.442	1.00 20.35	O
	ATOM	114	CB	THR	B	266	10.348	-33.803	-22.140	1.00 22.35	C
	ATOM	115	OG1	THR	B	266	9.061	-34.087	-21.583	1.00 24.46	O
	ATOM	116	CG2	THR	B	266	10.945	-32.573	-21.444	1.00 24.00	C
	ATOM	117	N	VAL	B	267	12.427	-34.075	-24.461	1.00 20.46	N
	ATOM	118	CA	VAL	B	267	13.730	-33.762	-25.023	1.00 21.11	C
	ATOM	119	C	VAL	B	267	13.548	-33.138	-26.416	1.00 21.34	C
	ATOM	120	O	VAL	B	267	14.188	-32.135	-26.747	1.00 19.99	O
	ATOM	121	CB	VAL	B	267	14.614	-35.039	-25.114	1.00 21.54	C
	ATOM	122	CG1	VAL	B	267	15.903	-34.740	-25.865	1.00 20.72	C
	ATOM	123	CG2	VAL	B	267	14.938	-35.541	-23.708	1.00 20.45	C
	ATOM	124	N	SER	B	268	12.663	-33.717	-27.222	1.00 21.61	N
	ATOM	125	CA	SER	B	268	12.411	-33.191	-28.567	1.00 21.96	C
	ATOM	126	C	SER	B	268	11.817	-31.790	-28.519	1.00 21.81	C
	ATOM	127	O	SER	B	268	12.158	-30.933	-29.336	1.00 22.60	O
	ATOM	128	CB	SER	B	268	11.474	-34.121	-29.344	1.00 21.57	C
	ATOM	129	OG	SER	B	268	12.141	-35.316	-29.721	1.00 24.06	O
	ATOM	130	N	GLU	B	269	10.928	-31.563	-27.557	1.00 21.64	N
	ATOM	131	CA	GLU	B	269	10.282	-30.272	-27.378	1.00 21.95	C

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ATOM    132  C   GLU B 269      11.321 -29.214 -26.999  1.00 21.68           C
ATOM    133  O   GLU B 269      11.301 -28.095 -27.518  1.00 18.12           O
ATOM    134  CB  GLU B 269       9.213 -30.399 -26.292  1.00 24.72           C
ATOM    135  CG  GLU B 269       8.480 -29.128 -25.940  1.00 27.67           C
ATOM    136  CD  GLU B 269       7.385 -29.380 -24.908  1.00 30.05           C
ATOM    137  OE1 GLU B 269       6.325 -29.915 -25.287  1.00 31.50           O
ATOM    138  OE2 GLU B 269       7.591 -29.057 -23.719  1.00 29.84           O
ATOM    139  N   ILE B 270      12.224 -29.581 -26.092  1.00 19.43           N
ATOM    140  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62           C
ATOM    141  C   ILE B 270      14.214 -28.314 -26.806  1.00 20.58           C
ATOM    142  O   ILE B 270      14.595 -27.151 -26.954  1.00 20.50           O
ATOM    143  CB  ILE B 270      14.157 -29.391 -24.533  1.00 20.30           C
ATOM    144  CG1 ILE B 270      13.337 -29.574 -23.254  1.00 21.32           C
ATOM    145  CG2 ILE B 270      15.415 -28.595 -24.266  1.00 19.17           C
ATOM    146  CD1 ILE B 270      12.926 -28.291 -22.583  1.00 23.40           C
ATOM    147  N   ALA B 277      19.316 -27.110 -21.396  1.00 17.01           N
ATOM    148  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80           C
ATOM    149  C   ALA B 277      19.591 -28.526 -19.382  1.00 17.37           C
ATOM    150  O   ALA B 277      20.710 -28.891 -19.755  1.00 17.09           O
ATOM    151  CB  ALA B 277      17.641 -28.805 -20.895  1.00 17.01           C
ATOM    152  N   LEU B 278      19.147 -28.673 -18.138  1.00 17.14           N
ATOM    153  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48           C
ATOM    154  C   LEU B 278      18.884 -30.535 -16.898  1.00 19.62           C
ATOM    155  O   LEU B 278      17.870 -30.330 -16.218  1.00 20.77           O
ATOM    156  CB  LEU B 278      20.140 -28.619 -15.869  1.00 19.19           C
ATOM    157  CG  LEU B 278      21.084 -29.308 -14.868  1.00 20.85           C
ATOM    158  CD1 LEU B 278      21.283 -28.411 -13.668  1.00 21.11           C
ATOM    159  CD2 LEU B 278      20.497 -30.647 -14.433  1.00 19.16           C
ATOM    160  N   PHE B 279      19.149 -31.691 -17.495  1.00 19.50           N
ATOM    161  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59           C
ATOM    162  C   PHE B 279      18.525 -33.709 -16.167  1.00 22.86           C
ATOM    163  O   PHE B 279      19.671 -34.065 -15.871  1.00 23.32           O
ATOM    164  CB  PHE B 279      18.385 -33.700 -18.651  1.00 21.07           C
ATOM    165  CG  PHE B 279      17.740 -33.099 -19.876  1.00 19.35           C
ATOM    166  CD1 PHE B 279      18.481 -32.898 -21.035  1.00 19.42           C
ATOM    167  CD2 PHE B 279      16.379 -32.794 -19.888  1.00 18.16           C
ATOM    168  CE1 PHE B 279      17.874 -32.405 -22.203  1.00 19.06           C
ATOM    169  CE2 PHE B 279      15.759 -32.298 -21.052  1.00 17.65           C
ATOM    170  CZ  PHE B 279      16.515 -32.108 -22.208  1.00 15.61           C
ATOM    171  N   VAL B 280      17.445 -34.037 -15.461  1.00 23.88           N
ATOM    172  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67           C
ATOM    173  C   VAL B 280      16.690 -36.136 -14.658  1.00 25.65           C
ATOM    174  O   VAL B 280      15.509 -36.239 -14.346  1.00 24.57           O
ATOM    175  CB  VAL B 280      16.883 -34.223 -13.048  1.00 26.89           C
ATOM    176  CG1 VAL B 280      16.954 -35.159 -11.847  1.00 28.12           C
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ATOM    177  CG2 VAL B 280      17.631 -32.929 -12.742  1.00 27.70           C
ATOM    178  N   PRO B 281      17.324 -37.080 -15.370  1.00 27.08           N
ATOM    179  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05           C
ATOM    180  C   PRO B 281      16.092 -39.121 -14.684  1.00 31.51           C
ATOM    181  O   PRO B 281      16.675 -39.223 -13.603  1.00 32.26           O
ATOM    182  CB  PRO B 281      17.851 -39.071 -16.492  1.00 29.44           C
ATOM    183  CG  PRO B 281      18.791 -37.992 -16.895  1.00 29.67           C
ATOM    184  CD  PRO B 281      18.750 -37.057 -15.726  1.00 27.31           C
ATOM    185  N   PHE B 282      14.908 -39.668 -14.923  1.00 33.83           N
ATOM    186  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13           C
ATOM    187  C   PHE B 282      15.078 -41.776 -13.880  1.00 38.09           C
ATOM    188  O   PHE B 282      15.357 -42.373 -14.921  1.00 38.33           O
ATOM    189  CB  PHE B 282      12.818 -40.808 -14.372  1.00 38.38           C
ATOM    190  CG  PHE B 282      12.032 -41.606 -13.377  1.00 40.57           C
ATOM    191  CD1 PHE B 282      11.720 -41.074 -12.130  1.00 41.80           C
ATOM    192  CD2 PHE B 282      11.590 -42.886 -13.689  1.00 41.65           C
ATOM    193  CE1 PHE B 282      10.975 -41.806 -11.209  1.00 42.03           C
ATOM    194  CE2 PHE B 282      10.843 -43.628 -12.773  1.00 42.49           C
ATOM    195  CZ  PHE B 282      10.536 -43.085 -11.532  1.00 41.74           C
ATOM    196  N   GLN B 288      16.212 -45.321 -19.533  1.00 30.94           N
ATOM    197  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77           C
ATOM    198  C   GLN B 288      15.783 -43.291 -20.885  1.00 29.70           C
ATOM    199  O   GLN B 288      16.268 -42.801 -21.902  1.00 29.79           O
ATOM    200  CB  GLN B 288      14.143 -45.158 -20.810  1.00 30.59           C
ATOM    201  CG  GLN B 288      13.473 -44.772 -22.109  1.00 29.73           C
ATOM    202  CD  GLN B 288      11.981 -44.971 -22.044  1.00 28.04           C
ATOM    203  OE1 GLN B 288      11.294 -44.295 -21.279  1.00 29.59           O
ATOM    204  NE2 GLN B 288      11.468 -45.905 -22.838  1.00 26.98           N
ATOM    205  N   GLN B 289      15.378 -42.554 -19.857  1.00 29.38           N
ATOM    206  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46           C
ATOM    207  C   GLN B 289      16.906 -40.613 -20.005  1.00 29.36           C
ATOM    208  O   GLN B 289      17.173 -39.557 -20.585  1.00 29.12           O
ATOM    209  CB  GLN B 289      14.772 -40.472 -18.700  1.00 29.25           C
ATOM    210  CG  GLN B 289      13.265 -40.416 -18.883  1.00 29.32           C
ATOM    211  CD  GLN B 289      12.575 -39.585 -17.826  1.00 29.84           C
ATOM    212  OE1 GLN B 289      13.191 -38.728 -17.188  1.00 29.52           O
ATOM    213  NE2 GLN B 289      11.281 -39.821 -17.647  1.00 28.95           N
ATOM    214  N   TYR B 290      17.835 -41.374 -19.442  1.00 28.95           N
ATOM    215  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55           C
ATOM    216  C   TYR B 290      19.593 -41.042 -21.032  1.00 28.80           C
ATOM    217  O   TYR B 290      20.192 -40.113 -21.567  1.00 29.22           O
ATOM    218  CB  TYR B 290      20.136 -41.934 -18.768  1.00 31.40           C
ATOM    219  CG  TYR B 290      21.587 -41.780 -19.148  1.00 33.37           C
ATOM    220  CD1 TYR B 290      22.332 -40.682 -18.717  1.00 34.57           C
ATOM    221  CD2 TYR B 290      22.192 -42.684 -20.017  1.00 34.90           C
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ATOM    222  CE1 TYR B 290      23.644 -40.490 -19.148  1.00 35.97           C
ATOM    223  CE2 TYR B 290      23.497 -42.500 -20.453  1.00 36.03           C
ATOM    224  CZ  TYR B 290      24.214 -41.402 -20.019  1.00 36.29           C
ATOM    225  OH  TYR B 290      25.499 -41.215 -20.475  1.00 39.44           O
ATOM    226  N   ASN B 292      17.658 -40.779 -23.508  1.00 25.52           N
ATOM    227  CA  ASN B 292      16.902 -39.784 -24.270  1.00 26.06           C
ATOM    228  C   ASN B 292      17.605 -38.427 -24.258  1.00 25.99           C
ATOM    229  O   ASN B 292      17.566 -37.687 -25.244  1.00 26.18           O
ATOM    230  CB  ASN B 292      15.484 -39.599 -23.709  1.00 24.78           C
ATOM    231  CG  ASN B 292      14.590 -40.811 -23.928  1.00 24.46           C
ATOM    232  OD1 ASN B 292      14.842 -41.641 -24.798  1.00 25.33           O
ATOM    233  ND2 ASN B 292      13.523 -40.900 -23.146  1.00 23.83           N
ATOM    234  N   ALA B 293      18.242 -38.105 -23.139  1.00 25.66           N
ATOM    235  CA  ALA B 293      18.926 -36.822 -22.979  1.00 25.69           C
ATOM    236  C   ALA B 293      20.346 -36.800 -23.521  1.00 25.67           C
ATOM    237  O   ALA B 293      20.855 -35.743 -23.902  1.00 25.52           O
ATOM    238  CB  ALA B 293      18.940 -36.422 -21.506  1.00 24.17           C
ATOM    239  N   LEU B 296      21.375 -34.703 -26.688  1.00 25.66           N
ATOM    240  CA  LEU B 296      21.521 -33.265 -26.481  1.00 25.42           C
ATOM    241  C   LEU B 296      22.784 -32.935 -25.688  1.00 26.07           C
ATOM    242  O   LEU B 296      23.435 -31.917 -25.944  1.00 25.26           O
ATOM    243  CB  LEU B 296      20.283 -32.685 -25.779  1.00 24.45           C
ATOM    244  CG  LEU B 296      19.066 -32.458 -26.679  1.00 25.59           C
ATOM    245  CD1 LEU B 296      17.968 -31.718 -25.911  1.00 23.56           C
ATOM    246  CD2 LEU B 296      19.496 -31.630 -27.893  1.00 25.87           C
ATOM    247  N   ALA B 302      23.066 -29.504 -23.507  1.00 20.94           N
ATOM    248  CA  ALA B 302      22.516 -29.770 -22.186  1.00 21.78           C
ATOM    249  C   ALA B 302      23.503 -30.507 -21.288  1.00 22.69           C
ATOM    250  O   ALA B 302      24.561 -30.948 -21.739  1.00 22.25           O
ATOM    251  CB  ALA B 302      21.243 -30.595 -22.327  1.00 20.10           C
ATOM    252  N   LYS B 303      23.156 -30.613 -20.009  1.00 24.62           N
ATOM    253  CA  LYS B 303      23.979 -31.340 -19.048  1.00 25.86           C
ATOM    254  C   LYS B 303      23.083 -32.319 -18.302  1.00 26.41           C
ATOM    255  O   LYS B 303      22.015 -31.948 -17.802  1.00 25.76           O
ATOM    256  CB  LYS B 303      24.632 -30.401 -18.036  1.00 27.85           C
ATOM    257  CG  LYS B 303      25.466 -31.146 -16.986  1.00 29.37           C
ATOM    258  CD  LYS B 303      26.150 -30.186 -16.025  1.00 32.41           C
ATOM    259  CE  LYS B 303      27.083 -30.912 -15.056  1.00 33.22           C
ATOM    260  NZ  LYS B 303      27.827 -29.952 -14.181  1.00 33.62           N
ATOM    261  N   ILE B 304      23.520 -33.570 -18.234  1.00 25.65           N
ATOM    262  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17           C
ATOM    263  C   ILE B 304      23.308 -34.855 -16.160  1.00 27.00           C
ATOM    264  O   ILE B 304      24.511 -35.012 -15.986  1.00 27.46           O
ATOM    265  CB  ILE B 304      22.786 -35.946 -18.316  1.00 27.06           C
ATOM    266  CG1 ILE B 304      22.242 -35.769 -19.733  1.00 27.61           C
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	ATOM	267	CG2	ILE	B	304	21.977	-36.996	-17.555	1.00	28.49	C
	ATOM	268	CD1	ILE	B	304	22.380	-37.009	-20.599	1.00	27.05	C
	ATOM	269	N	ILE	B	305	22.428	-34.869	-15.168	1.00	27.22	N
	ATOM	270	CA	ILE	B	305	22.843	-35.178	-13.813	1.00	29.01	C
5	ATOM	271	C	ILE	B	305	21.934	-36.302	-13.351	1.00	29.64	C
	ATOM	272	O	ILE	B	305	20.806	-36.067	-12.932	1.00	29.25	O
	ATOM	273	CB	ILE	B	305	22.713	-33.977	-12.858	1.00	28.91	C
	ATOM	274	CG1	ILE	B	305	23.660	-32.855	-13.299	1.00	29.51	C
	ATOM	275	CG2	ILE	B	305	23.063	-34.416	-11.432	1.00	30.98	C
10	ATOM	276	CD1	ILE	B	305	23.674	-31.653	-12.367	1.00	29.43	C
	TER											

TABLE 5 ATOMIC COORDINATES OF ACCEPTOR BINDING SITE

	REMARK	4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000									
15	ATOM	1	N	MET	B	12	-0.734	-48.902	-33.817	1.00	23.68	N
	ATOM	2	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	C
	ATOM	3	C	MET	B	12	0.361	-48.840	-31.720	1.00	25.31	C
	ATOM	4	O	MET	B	12	1.546	-48.645	-32.006	1.00	23.88	O
	ATOM	5	CB	MET	B	12	0.192	-51.019	-32.971	1.00	24.28	C
20	ATOM	6	CG	MET	B	12	-0.402	-51.726	-34.188	1.00	25.19	C
	ATOM	7	SD	MET	B	12	0.399	-53.284	-34.669	1.00	26.54	S
	ATOM	8	CE	MET	B	12	1.990	-52.691	-35.289	1.00	22.99	C
	ATOM	9	N	ALA	B	13	-0.224	-48.292	-30.657	1.00	27.08	N
	ATOM	10	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43	C
25	ATOM	11	C	ALA	B	13	-0.239	-47.192	-28.436	1.00	31.80	C
	ATOM	12	O	ALA	B	13	-1.143	-46.350	-28.352	1.00	32.16	O
	ATOM	13	CB	ALA	B	13	0.747	-46.074	-30.429	1.00	28.82	C
	ATOM	14	N	GLY	B	14	0.150	-47.934	-27.405	1.00	32.46	N
	ATOM	15	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82	C
30	ATOM	16	C	GLY	B	14	-0.107	-46.595	-25.299	1.00	34.82	C
	ATOM	17	O	GLY	B	14	0.975	-46.040	-25.479	1.00	35.47	O
	ATOM	18	N	GLY	B	15	-0.986	-46.188	-24.385	1.00	35.56	N
	ATOM	19	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08	C
	ATOM	20	C	GLY	B	15	0.539	-45.254	-22.683	1.00	36.84	C
35	ATOM	21	O	GLY	B	15	1.293	-44.311	-22.426	1.00	36.03	O
	ATOM	22	N	THR	B	16	0.755	-46.488	-22.240	1.00	36.65	N
	ATOM	23	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51	C
	ATOM	24	C	THR	B	16	3.158	-46.497	-22.264	1.00	38.35	C
	ATOM	25	O	THR	B	16	3.191	-46.798	-23.460	1.00	39.90	O
40	ATOM	26	CB	THR	B	16	1.926	-48.258	-20.974	1.00	38.51	C
	ATOM	27	OG1	THR	B	16	0.686	-48.558	-20.321	1.00	38.39	O
	ATOM	28	CG2	THR	B	16	3.075	-48.518	-20.005	1.00	39.11	C
	ATOM	29	N	GLY	B	17	4.168	-45.897	-21.649	1.00	37.68	N
	ATOM	30	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57	C

	ATOM	31	C	GLY	B	17	5.161	-44.303	-23.211	1.00 35.56	C
	ATOM	32	O	GLY	B	17	6.079	-43.843	-23.890	1.00 35.03	O
	ATOM	33	N	GLY	B	18	3.949	-43.752	-23.150	1.00 33.83	N
	ATOM	34	CA	GLY	B	18	3.631	-42.529	-23.872	1.00 33.48	C
	ATOM	35	C	GLY	B	18	3.825	-42.593	-25.378	1.00 33.12	C
	ATOM	36	O	GLY	B	18	4.345	-41.650	-25.984	1.00 35.38	O
	ATOM	37	N	HIS	B	19	3.416	-43.699	-25.988	1.00 30.26	N
	ATOM	38	CA	HIS	B	19	3.548	-43.865	-27.435	1.00 28.22	C
	ATOM	39	C	HIS	B	19	2.280	-43.370	-28.144	1.00 27.91	C
	ATOM	40	O	HIS	B	19	2.300	-43.049	-29.337	1.00 26.91	O
	ATOM	41	CB	HIS	B	19	3.772	-45.349	-27.779	1.00 25.81	C
	ATOM	42	CG	HIS	B	19	4.957	-45.966	-27.094	1.00 25.35	C
	ATOM	43	ND1	HIS	B	19	4.845	-47.025	-26.217	1.00 24.57	N
	ATOM	44	CD2	HIS	B	19	6.281	-45.694	-27.184	1.00 24.18	C
	ATOM	45	CE1	HIS	B	19	6.046	-47.380	-25.798	1.00 23.08	C
	ATOM	46	NE2	HIS	B	19	6.936	-46.589	-26.369	1.00 25.51	N
	ATOM	47	N	VAL	B	20	1.180	-43.310	-27.402	1.00 27.65	N
	ATOM	48	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00 27.77	C
	ATOM	49	C	VAL	B	20	-0.140	-41.452	-28.470	1.00 27.57	C
	ATOM	50	O	VAL	B	20	-0.771	-41.172	-29.486	1.00 27.12	O
	ATOM	51	CB	VAL	B	20	-1.248	-43.080	-26.942	1.00 28.57	C
	ATOM	52	CG1	VAL	B	20	-1.082	-42.114	-25.787	1.00 30.03	C
	ATOM	53	CG2	VAL	B	20	-2.602	-42.873	-27.631	1.00 26.82	C
	ATOM	54	N	LEU	B	40	-5.323	-50.004	-32.549	1.00 25.21	N
	ATOM	55	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00 24.71	C
	ATOM	56	C	LEU	B	40	-4.535	-51.235	-30.655	1.00 23.33	C
	ATOM	57	O	LEU	B	40	-3.387	-50.824	-30.563	1.00 23.43	O
	ATOM	58	CB	LEU	B	40	-4.326	-52.221	-32.952	1.00 25.21	C
	ATOM	59	CG	LEU	B	40	-4.416	-53.754	-32.868	1.00 26.95	C
	ATOM	60	CD1	LEU	B	40	-3.037	-54.334	-32.571	1.00 27.63	C
	ATOM	61	CD2	LEU	B	40	-5.421	-54.179	-31.817	1.00 26.69	C
	ATOM	62	N	GLU	B	47	-4.976	-45.941	-23.678	1.00 32.85	N
	ATOM	63	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00 31.79	C
	ATOM	64	C	GLU	B	47	-6.938	-46.017	-25.191	1.00 31.81	C
	ATOM	65	O	GLU	B	47	-7.626	-45.476	-26.055	1.00 31.31	O
	ATOM	66	CB	GLU	B	47	-4.624	-46.402	-26.080	1.00 30.62	C
	ATOM	67	CG	GLU	B	47	-4.755	-47.922	-26.051	1.00 29.85	C
	ATOM	68	CD	GLU	B	47	-3.793	-48.597	-25.082	1.00 29.78	C
	ATOM	69	OE1	GLU	B	47	-3.188	-47.895	-24.247	1.00 28.76	O
	ATOM	70	OE2	GLU	B	47	-3.649	-49.840	-25.156	1.00 29.01	O
	ATOM	71	N	ILE	B	63	-3.428	-59.342	-24.313	1.00 30.07	N
	ATOM	72	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00 31.38	C
	ATOM	73	C	ILE	B	63	-1.623	-59.981	-22.775	1.00 33.08	C
	ATOM	74	O	ILE	B	63	-0.444	-59.872	-22.430	1.00 33.21	O
	ATOM	75	CB	ILE	B	63	-1.081	-58.745	-24.883	1.00 30.06	C

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ATOM    76  CG1 ILE B  63      -1.143 -57.411 -24.137  1.00 29.94      C
ATOM    77  CG2 ILE B  63      -1.442 -58.567 -26.353  1.00 30.41      C
ATOM    78  CD1 ILE B  63      -0.128 -56.384 -24.632  1.00 29.62      C
ATOM    79  N   ARG B  67       2.953 -59.185 -21.440  1.00 31.54      N
ATOM    80  CA  ARG B  67       3.671 -57.928 -21.277  1.00 30.90      C
ATOM    81  C   ARG B  67       5.071 -58.142 -20.713  1.00 29.99      C
ATOM    82  O   ARG B  67       5.294 -59.034 -19.889  1.00 28.67      O
ATOM    83  CB  ARG B  67       2.888 -56.984 -20.363  1.00 32.28      C
ATOM    84  CG  ARG B  67       1.540 -56.576 -20.913  1.00 34.65      C
ATOM    85  CD  ARG B  67       0.926 -55.440 -20.097  1.00 36.69      C
ATOM    86  NE  ARG B  67      -0.259 -54.889 -20.748  1.00 38.28      N
ATOM    87  CZ  ARG B  67      -1.425 -55.519 -20.853  1.00 39.05      C
ATOM    88  NH1 ARG B  67      -1.583 -56.734 -20.341  1.00 39.61      N
ATOM    89  NH2 ARG B  67      -2.434 -54.935 -21.487  1.00 39.52      N
ATOM    90  N   GLY B  68       6.014 -57.321 -21.165  1.00 27.75      N
ATOM    91  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79      C
ATOM    92  C   GLY B  68       8.166 -58.579 -21.280  1.00 25.41      C
ATOM    93  O   GLY B  68       9.326 -58.779 -20.943  1.00 26.04      O
ATOM    94  N   GLY B 102       3.556 -48.986 -35.936  1.00 20.96      N
ATOM    95  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23      C
ATOM    96  C   GLY B 102       4.655 -48.282 -33.918  1.00 18.45      C
ATOM    97  O   GLY B 102       5.765 -48.016 -34.381  1.00 18.70      O
ATOM    98  N   MET B 103       4.155 -47.660 -32.857  1.00 18.01      N
ATOM    99  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93      C
ATOM   100  C   MET B 103       5.612 -47.128 -30.957  1.00 18.98      C
ATOM   101  O   MET B 103       6.134 -46.357 -30.158  1.00 17.96      O
ATOM   102  CB  MET B 103       3.928 -45.477 -31.781  1.00 20.02      C
ATOM   103  CG  MET B 103       3.121 -44.888 -32.944  1.00 21.61      C
ATOM   104  SD  MET B 103       4.212 -44.135 -34.157  1.00 23.45      S
ATOM   105  CE  MET B 103       4.718 -42.680 -33.271  1.00 21.40      C
ATOM   106  N   GLY B 104       5.640 -48.450 -30.827  1.00 21.56      N
ATOM   107  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89      C
ATOM   108  C   GLY B 104       5.192 -49.614 -28.764  1.00 23.28      C
ATOM   109  O   GLY B 104       4.009 -49.353 -28.980  1.00 22.50      O
ATOM   110  N   GLY B 105       5.583 -50.364 -27.741  1.00 23.01      N
ATOM   111  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54      C
ATOM   112  C   GLY B 105       4.358 -52.380 -27.078  1.00 23.17      C
ATOM   113  O   GLY B 105       4.449 -52.844 -28.214  1.00 22.69      O
ATOM   114  N   TYR B 106       4.018 -53.118 -26.026  1.00 22.87      N
ATOM   115  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37      C
ATOM   116  C   TYR B 106       2.719 -55.018 -27.100  1.00 20.52      C
ATOM   117  O   TYR B 106       2.867 -56.052 -27.746  1.00 20.50      O
ATOM   118  CB  TYR B 106       3.632 -55.181 -24.774  1.00 25.08      C
ATOM   119  CG  TYR B 106       4.864 -55.008 -23.929  1.00 28.19      C
ATOM   120  CD1 TYR B 106       4.869 -54.153 -22.830  1.00 31.96      C
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	ATOM	121	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00	31.27	C
	ATOM	122	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00	33.13	C
	ATOM	123	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00	32.27	C
	ATOM	124	CZ	TYR	B	106	7.219	-54.541	-22.487	1.00	33.19	C
	ATOM	125	OH	TYR	B	106	8.388	-54.291	-21.802	1.00	35.95	O
	ATOM	126	N	VAL	B	107	1.628	-54.270	-27.205	1.00	19.06	N
	ATOM	127	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06	C
	ATOM	128	C	VAL	B	107	1.015	-54.743	-29.559	1.00	17.45	C
	ATOM	129	O	VAL	B	107	0.502	-55.536	-30.346	1.00	16.99	O
	ATOM	130	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00	20.95	C
	ATOM	131	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00	21.39	C
	ATOM	132	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00	21.30	C
	ATOM	133	N	SER	B	108	1.991	-53.916	-29.918	1.00	17.96	N
	ATOM	134	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67	C
	ATOM	135	C	SER	B	108	3.197	-55.187	-31.694	1.00	20.38	C
	ATOM	136	O	SER	B	108	3.385	-55.449	-32.884	1.00	21.25	O
	ATOM	137	CB	SER	B	108	3.424	-52.691	-31.508	1.00	19.56	C
	ATOM	138	OG	SER	B	108	4.666	-52.824	-30.837	1.00	19.63	O
	ATOM	139	N	GLY	B	109	3.595	-55.995	-30.710	1.00	19.59	N
	ATOM	140	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03	C
	ATOM	141	C	GLY	B	109	3.311	-58.170	-31.792	1.00	19.61	C
	ATOM	142	O	GLY	B	109	3.579	-58.517	-32.940	1.00	19.24	O
	ATOM	143	N	PRO	B	110	2.206	-58.606	-31.173	1.00	19.20	N
	ATOM	144	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99	C
	ATOM	145	C	PRO	B	110	0.651	-58.761	-33.075	1.00	19.22	C
	ATOM	146	O	PRO	B	110	0.406	-59.371	-34.116	1.00	17.13	O
	ATOM	147	CB	PRO	B	110	0.198	-59.737	-30.778	1.00	20.41	C
	ATOM	148	CG	PRO	B	110	0.998	-59.720	-29.515	1.00	19.81	C
	ATOM	149	CD	PRO	B	110	1.914	-58.528	-29.729	1.00	19.94	C
	ATOM	150	N	HIS	B	125	8.182	-46.638	-35.447	1.00	21.40	N
	ATOM	151	CA	HIS	B	125	8.814	-45.413	-34.981	1.00	21.42	C
	ATOM	152	C	HIS	B	125	9.196	-45.642	-33.519	1.00	21.70	C
	ATOM	153	O	HIS	B	125	8.378	-46.117	-32.725	1.00	19.81	O
	ATOM	154	CB	HIS	B	125	7.858	-44.218	-35.067	1.00	21.57	C
	ATOM	155	CG	HIS	B	125	8.432	-42.948	-34.511	1.00	23.73	C
	ATOM	156	ND1	HIS	B	125	9.274	-42.127	-35.236	1.00	26.23	N
	ATOM	157	CD2	HIS	B	125	8.300	-42.368	-33.295	1.00	22.15	C
	ATOM	158	CE1	HIS	B	125	9.631	-41.095	-34.490	1.00	24.20	C
	ATOM	159	NE2	HIS	B	125	9.054	-41.218	-33.307	1.00	26.07	N
	ATOM	160	N	GLU	B	126	10.444	-45.332	-33.186	1.00	21.20	N
	ATOM	161	CA	GLU	B	126	10.947	-45.452	-31.817	1.00	22.15	C
	ATOM	162	C	GLU	B	126	11.205	-44.027	-31.326	1.00	21.93	C
	ATOM	163	O	GLU	B	126	12.016	-43.300	-31.908	1.00	21.33	O
	ATOM	164	CB	GLU	B	126	12.252	-46.246	-31.790	1.00	21.99	C
	ATOM	165	CG	GLU	B	126	12.958	-46.206	-30.439	1.00	22.04	C

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ATOM    166  CD  GLU B 126      12.119 -46.824 -29.338  1.00 21.43      C
ATOM    167  OE1 GLU B 126      11.767 -48.014 -29.471  1.00 21.92      O
ATOM    168  OE2 GLU B 126      11.807 -46.124 -28.349  1.00 21.08      O
ATOM    169  N   GLN B 127      10.520 -43.624 -30.259  1.00 22.62      N
ATOM    170  CA  GLN B 127      10.682 -42.270 -29.735  1.00 22.81      C
ATOM    171  C   GLN B 127      11.874 -42.087 -28.809  1.00 22.39      C
ATOM    172  O   GLN B 127      12.399 -40.976 -28.682  1.00 22.43      O
ATOM    173  CB  GLN B 127       9.414 -41.814 -28.989  1.00 23.56      C
ATOM    174  CG  GLN B 127       8.147 -41.783 -29.830  1.00 24.46      C
ATOM    175  CD  GLN B 127       7.312 -43.041 -29.687  1.00 25.85      C
ATOM    176  OE1 GLN B 127       6.842 -43.366 -28.591  1.00 23.78      O
ATOM    177  NE2 GLN B 127       7.119 -43.758 -30.797  1.00 24.91      N
ATOM    178  N   ASN B 128      12.314 -43.173 -28.177  1.00 22.35      N
ATOM    179  CA  ASN B 128      13.406 -43.097 -27.216  1.00 22.96      C
ATOM    180  C   ASN B 128      14.824 -43.314 -27.742  1.00 23.87      C
ATOM    181  O   ASN B 128      15.026 -43.856 -28.830  1.00 24.05      O
ATOM    182  CB  ASN B 128      13.136 -44.080 -26.064  1.00 22.85      C
ATOM    183  CG  ASN B 128      11.742 -43.919 -25.474  1.00 23.25      C
ATOM    184  OD1 ASN B 128      10.804 -44.632 -25.848  1.00 26.04      O
ATOM    185  ND2 ASN B 128      11.597 -42.975 -24.556  1.00 22.68      N
ATOM    186  N   GLY B 132      12.851 -49.814 -27.506  1.00 24.52      N
ATOM    187  CA  GLY B 132      12.007 -50.532 -26.568  1.00 24.05      C
ATOM    188  C   GLY B 132      12.150 -52.019 -26.831  1.00 23.35      C
ATOM    189  O   GLY B 132      12.582 -52.419 -27.904  1.00 22.89      O
ATOM    190  N   LEU B 133      11.788 -52.846 -25.860  1.00 23.38      N
ATOM    191  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54      C
ATOM    192  C   LEU B 133      11.209 -54.833 -27.276  1.00 22.84      C
ATOM    193  O   LEU B 133      11.784 -55.619 -28.027  1.00 21.86      O
ATOM    194  CB  LEU B 133      11.328 -54.996 -24.786  1.00 25.48      C
ATOM    195  CG  LEU B 133      11.388 -56.527 -24.780  1.00 27.50      C
ATOM    196  CD1 LEU B 133      12.840 -56.984 -24.866  1.00 28.69      C
ATOM    197  CD2 LEU B 133      10.735 -57.059 -23.509  1.00 28.04      C
ATOM    198  N   THR B 134       9.975 -54.401 -27.499  1.00 21.72      N
ATOM    199  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22      C
ATOM    200  C   THR B 134       9.693 -54.326 -29.986  1.00 20.62      C
ATOM    201  O   THR B 134       9.843 -55.091 -30.932  1.00 20.33      O
ATOM    202  CB  THR B 134       7.716 -54.509 -28.449  1.00 20.99      C
ATOM    203  OG1 THR B 134       7.257 -55.075 -27.210  1.00 20.94      O
ATOM    204  CG2 THR B 134       6.872 -55.073 -29.600  1.00 20.64      C
ATOM    205  N   ASN B 135       9.932 -53.021 -30.075  1.00 21.24      N
ATOM    206  CA  ASN B 135      10.407 -52.419 -31.324  1.00 20.50      C
ATOM    207  C   ASN B 135      11.724 -53.064 -31.767  1.00 20.78      C
ATOM    208  O   ASN B 135      11.945 -53.290 -32.953  1.00 20.41      O
ATOM    209  CB  ASN B 135      10.637 -50.911 -31.142  1.00 19.58      C
ATOM    210  CG  ASN B 135       9.457 -50.058 -31.597  1.00 19.93      C
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ATOM	211	OD1	ASN	B	135	9.454	-48.837	-31.390	1.00	21.78	O
ATOM	212	ND2	ASN	B	135	8.467	-50.677	-32.219	1.00	17.21	N
ATOM	213	N	LEU	B	138	10.741	-56.381	-33.386	1.00	21.61	N
ATOM	214	CA	LEU	B	138	9.744	-56.188	-34.431	1.00	23.15	C
ATOM	215	C	LEU	B	138	10.384	-55.558	-35.676	1.00	23.07	C
ATOM	216	O	LEU	B	138	9.958	-55.801	-36.809	1.00	22.68	O
ATOM	217	CB	LEU	B	138	8.618	-55.305	-33.886	1.00	23.87	C
ATOM	218	CG	LEU	B	138	7.312	-55.155	-34.664	1.00	26.48	C
ATOM	219	CD1	LEU	B	138	6.672	-56.508	-34.915	1.00	25.34	C
ATOM	220	CD2	LEU	B	138	6.383	-54.267	-33.851	1.00	25.90	C

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TABLE 6 ATOMIC COORDINATES OF MEMBRANE ASSOCIATION SITE

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REMARK   4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   MET B  12      -0.734 -48.902 -33.817  1.00 23.68      N
ATOM      2  CA  MET B  12      -0.523 -49.707 -32.613  1.00 24.54      C
ATOM      3  C   MET B  12       0.361 -48.840 -31.720  1.00 25.31      C
ATOM      4  O   MET B  12       1.546 -48.645 -32.006  1.00 23.88      O
ATOM      5  CB  MET B  12       0.192 -51.019 -32.971  1.00 24.28      C
ATOM      6  CG  MET B  12      -0.402 -51.726 -34.188  1.00 25.19      C
ATOM      7  SD  MET B  12       0.399 -53.284 -34.669  1.00 26.54      S
ATOM      8  CE  MET B  12       1.990 -52.691 -35.289  1.00 22.99      C
ATOM      9  N   LEU B  40      -5.323 -50.004 -32.549  1.00 25.21      N
ATOM     10  CA  LEU B  40      -5.200 -51.364 -32.026  1.00 24.71      C
ATOM     11  C   LEU B  40      -4.535 -51.235 -30.655  1.00 23.33      C
ATOM     12  O   LEU B  40      -3.387 -50.824 -30.563  1.00 23.43      O
ATOM     13  CB  LEU B  40      -4.326 -52.221 -32.952  1.00 25.21      C
ATOM     14  CG  LEU B  40      -4.416 -53.754 -32.868  1.00 26.95      C
ATOM     15  CD1 LEU B  40      -3.037 -54.334 -32.571  1.00 27.63      C
ATOM     16  CD2 LEU B  40      -5.421 -54.179 -31.817  1.00 26.69      C
ATOM     17  N   ILE B  61      -7.271 -56.229 -28.295  1.00 29.38      N
ATOM     18  CA  ILE B  61      -6.832 -57.616 -28.269  1.00 28.55      C
ATOM     19  C   ILE B  61      -6.344 -57.855 -26.848  1.00 29.13      C
ATOM     20  O   ILE B  61      -6.124 -56.906 -26.091  1.00 28.80      O
ATOM     21  CB  ILE B  61      -5.674 -57.923 -29.258  1.00 28.48      C
ATOM     22  CG1 ILE B  61      -4.422 -57.126 -28.892  1.00 26.70      C
ATOM     23  CG2 ILE B  61      -6.123 -57.650 -30.694  1.00 27.65      C
ATOM     24  CD1 ILE B  61      -3.177 -57.615 -29.638  1.00 27.03      C
ATOM     25  N   ARG B  62      -6.186 -59.116 -26.473  1.00 29.38      N
ATOM     26  CA  ARG B  62      -5.709 -59.416 -25.133  1.00 30.76      C
ATOM     27  C   ARG B  62      -4.274 -59.923 -25.156  1.00 29.32      C
ATOM     28  O   ARG B  62      -3.933 -60.809 -25.934  1.00 28.65      O
ATOM     29  CB  ARG B  62      -6.630 -60.447 -24.461  1.00 32.36      C
ATOM     30  CG  ARG B  62      -6.130 -60.955 -23.114  1.00 35.99      C
ATOM     31  CD  ARG B  62      -5.438 -59.859 -22.311  1.00 37.86      C
ATOM     32  NE  ARG B  62      -6.297 -58.718 -22.004  1.00 40.01      N
ATOM     33  CZ  ARG B  62      -5.840 -57.504 -21.711  1.00 39.09      C
ATOM     34  NH1 ARG B  62      -4.536 -57.275 -21.690  1.00 39.24      N
ATOM     35  NH2 ARG B  62      -6.686 -56.518 -21.439  1.00 40.03      N
ATOM     36  N   ILE B  63      -3.428 -59.342 -24.313  1.00 30.07      N
ATOM     37  CA  ILE B  63      -2.036 -59.770 -24.231  1.00 31.38      C
ATOM     38  C   ILE B  63      -1.623 -59.981 -22.775  1.00 33.08      C
ATOM     39  O   ILE B  63      -0.444 -59.872 -22.430  1.00 33.21      O
ATOM     40  CB  ILE B  63      -1.081 -58.745 -24.883  1.00 30.06      C
ATOM     41  CG1 ILE B  63      -1.143 -57.411 -24.137  1.00 29.94      C
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	ATOM	42	CG2	ILE	B	63	-1.442	-58.567	-26.353	1.00 30.41	C
	ATOM	43	CD1	ILE	B	63	-0.128	-56.384	-24.632	1.00 29.62	C
	ATOM	44	N	SER	B	64	-2.603	-60.284	-21.927	1.00 35.38	N
	ATOM	45	CA	SER	B	64	-2.356	-60.520	-20.505	1.00 37.51	C
	ATOM	46	C	SER	B	64	-1.326	-61.622	-20.311	1.00 37.32	C
	ATOM	47	O	SER	B	64	-1.411	-62.682	-20.933	1.00 37.86	O
	ATOM	48	CB	SER	B	64	-3.652	-60.912	-19.792	1.00 38.82	C
	ATOM	49	OG	SER	B	64	-4.558	-59.823	-19.750	1.00 42.88	O
	ATOM	50	N	GLY	B	65	-0.356	-61.370	-19.441	1.00 37.81	N
	ATOM	51	CA	GLY	B	65	0.679	-62.355	-19.199	1.00 37.13	C
	ATOM	52	C	GLY	B	65	1.798	-62.283	-20.226	1.00 36.76	C
	ATOM	53	O	GLY	B	65	2.858	-62.889	-20.038	1.00 37.57	O
	ATOM	54	N	LEU	B	66	1.577	-61.539	-21.307	1.00 34.63	N
	ATOM	55	CA	LEU	B	66	2.591	-61.413	-22.355	1.00 33.17	C
	ATOM	56	C	LEU	B	66	3.414	-60.133	-22.246	1.00 32.72	C
	ATOM	57	O	LEU	B	66	4.451	-60.002	-22.893	1.00 33.13	O
	ATOM	58	CB	LEU	B	66	1.936	-61.470	-23.735	1.00 32.08	C
	ATOM	59	CG	LEU	B	66	1.162	-62.747	-24.061	1.00 32.52	C
	ATOM	60	CD1	LEU	B	66	0.563	-62.626	-25.445	1.00 31.38	C
	ATOM	61	CD2	LEU	B	66	2.093	-63.957	-23.984	1.00 31.67	C
	ATOM	62	N	ARG	B	67	2.953	-59.185	-21.440	1.00 31.54	N
	ATOM	63	CA	ARG	B	67	3.671	-57.928	-21.277	1.00 30.90	C
	ATOM	64	C	ARG	B	67	5.071	-58.142	-20.713	1.00 29.99	C
	ATOM	65	O	ARG	B	67	5.294	-59.034	-19.889	1.00 28.67	O
	ATOM	66	CB	ARG	B	67	2.888	-56.984	-20.363	1.00 32.28	C
	ATOM	67	CG	ARG	B	67	1.540	-56.576	-20.913	1.00 34.65	C
	ATOM	68	CD	ARG	B	67	0.926	-55.440	-20.097	1.00 36.69	C
	ATOM	69	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00 38.28	N
	ATOM	70	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00 39.05	C
	ATOM	71	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00 39.61	N
	ATOM	72	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00 39.52	N
	ATOM	73	N	GLY	B	68	6.014	-57.321	-21.165	1.00 27.75	N
	ATOM	74	CA	GLY	B	68	7.380	-57.427	-20.685	1.00 26.79	C
	ATOM	75	C	GLY	B	68	8.166	-58.579	-21.280	1.00 25.41	C
	ATOM	76	O	GLY	B	68	9.326	-58.779	-20.943	1.00 26.04	O
	ATOM	77	N	LYS	B	69	7.546	-59.342	-22.170	1.00 24.55	N
	ATOM	78	CA	LYS	B	69	8.238	-60.463	-22.796	1.00 23.93	C
	ATOM	79	C	LYS	B	69	8.825	-60.062	-24.142	1.00 23.32	C
	ATOM	80	O	LYS	B	69	8.151	-59.404	-24.944	1.00 21.96	O
	ATOM	81	CB	LYS	B	69	7.284	-61.641	-23.033	1.00 24.12	C
	ATOM	82	CG	LYS	B	69	6.757	-62.360	-21.794	1.00 25.08	C
	ATOM	83	CD	LYS	B	69	5.887	-63.553	-22.224	1.00 25.44	C
	ATOM	84	CE	LYS	B	69	5.357	-64.358	-21.035	1.00 28.31	C
	ATOM	85	NZ	LYS	B	69	6.468	-64.877	-20.175	1.00 29.71	N
	ATOM	86	N	GLY	B	70	10.075	-60.470	-24.374	1.00 22.48	N

ATOM	87	CA	GLY	B	70	10.755	-60.229	-25.636	1.00	22.26	C
ATOM	88	C	GLY	B	70	10.308	-61.337	-26.588	1.00	22.17	C
ATOM	89	O	GLY	B	70	9.512	-62.183	-26.195	1.00	21.62	O
ATOM	90	N	ILE	B	71	10.819	-61.373	-27.814	1.00	21.85	N
ATOM	91	CA	ILE	B	71	10.357	-62.386	-28.762	1.00	23.55	C
ATOM	92	C	ILE	B	71	10.616	-63.840	-28.359	1.00	23.88	C
ATOM	93	O	ILE	B	71	9.775	-64.707	-28.592	1.00	21.66	O
ATOM	94	CB	ILE	B	71	10.926	-62.142	-30.181	1.00	23.52	C
ATOM	95	CG1	ILE	B	71	10.264	-63.096	-31.182	1.00	24.18	C
ATOM	96	CG2	ILE	B	71	12.435	-62.375	-30.192	1.00	25.96	C
ATOM	97	CD1	ILE	B	71	8.745	-62.981	-31.263	1.00	25.73	C
ATOM	98	N	LYS	B	72	11.764	-64.119	-27.751	1.00	23.82	N
ATOM	99	CA	LYS	B	72	12.038	-65.491	-27.343	1.00	24.92	C
ATOM	100	C	LYS	B	72	11.068	-65.925	-26.245	1.00	23.73	C
ATOM	101	O	LYS	B	72	10.592	-67.062	-26.245	1.00	24.08	O
ATOM	102	CB	LYS	B	72	13.491	-65.634	-26.875	1.00	26.86	C
ATOM	103	CG	LYS	B	72	14.496	-65.590	-28.019	1.00	31.29	C
ATOM	104	CD	LYS	B	72	15.925	-65.791	-27.518	1.00	36.00	C
ATOM	105	CE	LYS	B	72	16.926	-65.816	-28.671	1.00	38.82	C
ATOM	106	NZ	LYS	B	72	18.342	-65.957	-28.192	1.00	41.21	N
ATOM	107	N	ALA	B	73	10.765	-65.016	-25.322	1.00	21.62	N
ATOM	108	CA	ALA	B	73	9.839	-65.306	-24.233	1.00	21.18	C
ATOM	109	C	ALA	B	73	8.412	-65.454	-24.771	1.00	20.36	C
ATOM	110	O	ALA	B	73	7.619	-66.250	-24.267	1.00	18.97	O
ATOM	111	CB	ALA	B	73	9.895	-64.196	-23.187	1.00	22.25	C
ATOM	112	N	LEU	B	74	8.076	-64.673	-25.791	1.00	20.23	N
ATOM	113	CA	LEU	B	74	6.745	-64.762	-26.387	1.00	19.36	C
ATOM	114	C	LEU	B	74	6.549	-66.110	-27.069	1.00	19.37	C
ATOM	115	O	LEU	B	74	5.539	-66.779	-26.863	1.00	20.01	O
ATOM	116	CB	LEU	B	74	6.540	-63.643	-27.417	1.00	18.42	C
ATOM	117	CG	LEU	B	74	6.422	-62.208	-26.884	1.00	18.80	C
ATOM	118	CD1	LEU	B	74	6.473	-61.197	-28.039	1.00	19.86	C
ATOM	119	CD2	LEU	B	74	5.109	-62.071	-26.104	1.00	19.45	C
ATOM	120	N	ILE	B	75	7.520	-66.507	-27.883	1.00	20.59	N
ATOM	121	CA	ILE	B	75	7.434	-67.768	-28.601	1.00	21.18	C
ATOM	122	C	ILE	B	75	7.488	-68.942	-27.624	1.00	21.20	C
ATOM	123	O	ILE	B	75	7.125	-70.063	-27.979	1.00	21.59	O
ATOM	124	CB	ILE	B	75	8.571	-67.896	-29.641	1.00	22.95	C
ATOM	125	CG1	ILE	B	75	8.598	-66.657	-30.540	1.00	26.82	C
ATOM	126	CG2	ILE	B	75	8.334	-69.108	-30.527	1.00	25.38	C
ATOM	127	CD1	ILE	B	75	7.304	-66.442	-31.327	1.00	28.48	C
ATOM	128	N	ALA	B	76	7.940	-68.680	-26.399	1.00	20.49	N
ATOM	129	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72	C
ATOM	130	C	ALA	B	76	6.624	-69.904	-24.732	1.00	21.54	C
ATOM	131	O	ALA	B	76	6.441	-70.778	-23.875	1.00	20.75	O

ATOM	132	CB	ALA	B	76	9.026	-69.372	-24.305	1.00	21.92	C
ATOM	133	N	ALA	B	77	5.668	-69.066	-25.145	1.00	20.61	N
ATOM	134	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07	C
ATOM	135	C	ALA	B	77	3.383	-69.298	-25.881	1.00	21.69	C
ATOM	136	O	ALA	B	77	2.567	-68.430	-26.199	1.00	21.93	O
ATOM	137	CB	ALA	B	77	3.937	-67.830	-23.924	1.00	20.10	C
ATOM	138	N	PRO	B	78	3.507	-70.446	-26.564	1.00	22.38	N
ATOM	139	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95	C
ATOM	140	C	PRO	B	78	1.278	-70.535	-27.813	1.00	21.19	C
ATOM	141	O	PRO	B	78	0.789	-69.939	-28.776	1.00	19.68	O
ATOM	142	CB	PRO	B	78	3.027	-72.350	-27.861	1.00	22.21	C
ATOM	143	CG	PRO	B	78	4.288	-72.547	-27.117	1.00	24.07	C
ATOM	144	CD	PRO	B	78	4.211	-71.603	-25.976	1.00	21.89	C
ATOM	145	N	LEU	B	79	0.544	-70.961	-26.790	1.00	21.21	N
ATOM	146	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32	C
ATOM	147	C	LEU	B	79	-1.275	-69.263	-26.707	1.00	21.17	C
ATOM	148	O	LEU	B	79	-2.125	-68.800	-27.481	1.00	20.44	O
ATOM	149	CB	LEU	B	79	-1.569	-71.476	-25.630	1.00	20.99	C
ATOM	150	CG	LEU	B	79	-1.397	-72.988	-25.617	1.00	22.40	C
ATOM	151	CD1	LEU	B	79	-2.504	-73.619	-24.772	1.00	22.01	C
ATOM	152	CD2	LEU	B	79	-1.438	-73.521	-27.021	1.00	23.82	C
ATOM	153	N	ARG	B	80	-0.656	-68.529	-25.788	1.00	20.91	N
ATOM	154	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30	C
ATOM	155	C	ARG	B	80	-0.526	-66.233	-26.790	1.00	21.29	C
ATOM	156	O	ARG	B	80	-1.278	-65.355	-27.223	1.00	21.47	O
ATOM	157	CB	ARG	B	80	-0.444	-66.583	-24.312	1.00	22.12	C
ATOM	158	CG	ARG	B	80	-1.286	-67.051	-23.118	1.00	24.03	C
ATOM	159	CD	ARG	B	80	-0.610	-66.738	-21.807	1.00	23.42	C
ATOM	160	NE	ARG	B	80	0.581	-67.556	-21.610	1.00	24.59	N
ATOM	161	CZ	ARG	B	80	1.466	-67.351	-20.642	1.00	26.08	C
ATOM	162	NH1	ARG	B	80	1.290	-66.349	-19.787	1.00	26.92	N
ATOM	163	NH2	ARG	B	80	2.514	-68.152	-20.519	1.00	27.22	N
ATOM	164	N	ILE	B	81	0.683	-66.448	-27.303	1.00	19.29	N
ATOM	165	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47	C
ATOM	166	C	ILE	B	81	0.256	-65.937	-29.654	1.00	18.99	C
ATOM	167	O	ILE	B	81	-0.149	-65.028	-30.378	1.00	19.38	O
ATOM	168	CB	ILE	B	81	2.639	-65.793	-28.730	1.00	17.92	C
ATOM	169	CG1	ILE	B	81	3.067	-64.753	-29.769	1.00	18.63	C
ATOM	170	CG2	ILE	B	81	2.949	-67.200	-29.206	1.00	17.33	C
ATOM	171	CD1	ILE	B	81	2.746	-63.318	-29.346	1.00	17.46	C
ATOM	172	N	PHE	B	82	-0.056	-67.211	-29.880	1.00	19.39	N
ATOM	173	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15	C
ATOM	174	C	PHE	B	82	-2.250	-66.931	-30.959	1.00	19.94	C
ATOM	175	O	PHE	B	82	-2.777	-66.444	-31.970	1.00	19.64	O
ATOM	176	CB	PHE	B	82	-1.057	-69.103	-31.136	1.00	19.27	C

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ATOM    177  CG  PHE B  82     -1.811 -69.548 -32.368  1.00 19.87      C
ATOM    178  CD1 PHE B  82     -1.180 -69.602 -33.603  1.00 20.87      C
ATOM    179  CD2 PHE B  82     -3.154 -69.898 -32.289  1.00 21.11      C
ATOM    180  CE1 PHE B  82     -1.872 -70.002 -34.753  1.00 21.20      C
ATOM    181  CE2 PHE B  82     -3.857 -70.297 -33.429  1.00 22.26      C
ATOM    182  CZ  PHE B  82     -3.212 -70.349 -34.663  1.00 22.14      C
ATOM    183  N   ASN B  83     -2.832 -66.923 -29.764  1.00 19.29      N
ATOM    184  CA  ASN B  83     -4.150 -66.332 -29.577  1.00 20.90      C
ATOM    185  C   ASN B  83     -4.178 -64.821 -29.812  1.00 20.83      C
ATOM    186  O   ASN B  83     -5.086 -64.316 -30.472  1.00 21.92      O
ATOM    187  CB  ASN B  83     -4.693 -66.641 -28.178  1.00 20.55      C
ATOM    188  CG  ASN B  83     -6.158 -66.244 -28.028  1.00 22.79      C
ATOM    189  OD1 ASN B  83     -6.505 -65.374 -27.229  1.00 25.14      O
ATOM    190  ND2 ASN B  83     -7.018 -66.877 -28.807  1.00 20.47      N
ATOM    191  N   ALA B  84     -3.203 -64.092 -29.275  1.00 19.74      N
ATOM    192  CA  ALA B  84     -3.177 -62.647 -29.484  1.00 19.30      C
ATOM    193  C   ALA B  84     -2.967 -62.380 -30.981  1.00 19.94      C
ATOM    194  O   ALA B  84     -3.561 -61.459 -31.552  1.00 19.69      O
ATOM    195  CB  ALA B  84     -2.060 -62.008 -28.662  1.00 18.59      C
ATOM    196  N   TRP B  85     -2.118 -63.197 -31.603  1.00 19.77      N
ATOM    197  CA  TRP B  85     -1.820 -63.111 -33.032  1.00 20.56      C
ATOM    198  C   TRP B  85     -3.090 -63.354 -33.865  1.00 21.76      C
ATOM    199  O   TRP B  85     -3.339 -62.658 -34.859  1.00 20.40      O
ATOM    200  CB  TRP B  85     -0.754 -64.148 -33.396  1.00 21.46      C
ATOM    201  CG  TRP B  85     -0.365 -64.167 -34.856  1.00 23.00      C
ATOM    202  CD1 TRP B  85      0.301 -63.189 -35.548  1.00 23.17      C
ATOM    203  CD2 TRP B  85     -0.588 -65.232 -35.785  1.00 23.69      C
ATOM    204  NE1 TRP B  85      0.509 -63.585 -36.848  1.00 24.28      N
ATOM    205  CE2 TRP B  85     -0.024 -64.835 -37.022  1.00 24.14      C
ATOM    206  CE3 TRP B  85     -1.206 -66.486 -35.693  1.00 24.79      C
ATOM    207  CZ2 TRP B  85     -0.060 -65.650 -38.160  1.00 24.90      C
ATOM    208  CZ3 TRP B  85     -1.243 -67.299 -36.827  1.00 25.45      C
ATOM    209  CH2 TRP B  85     -0.671 -66.875 -38.045  1.00 25.15      C
ATOM    210  N   ARG B  86     -3.885 -64.346 -33.467  1.00 22.03      N
ATOM    211  CA  ARG B  86     -5.140 -64.660 -34.166  1.00 23.28      C
ATOM    212  C   ARG B  86     -6.151 -63.517 -34.007  1.00 22.98      C
ATOM    213  O   ARG B  86     -6.890 -63.195 -34.942  1.00 21.37      O
ATOM    214  CB  ARG B  86     -5.754 -65.965 -33.623  1.00 24.72      C
ATOM    215  CG  ARG B  86     -4.999 -67.236 -34.021  1.00 27.21      C
ATOM    216  CD  ARG B  86     -5.368 -67.725 -35.418  1.00 29.60      C
ATOM    217  NE  ARG B  86     -6.626 -68.477 -35.422  1.00 31.45      N
ATOM    218  CZ  ARG B  86     -7.185 -69.004 -36.508  1.00 31.37      C
ATOM    219  NH1 ARG B  86     -6.607 -68.862 -37.696  1.00 32.19      N
ATOM    220  NH2 ARG B  86     -8.314 -69.694 -36.405  1.00 31.39      N
ATOM    221  N   GLN B  87     -6.190 -62.916 -32.821  1.00 22.90      N
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ATOM	222	CA	GLN	B	87	-7.101	-61.802	-32.567	1.00	24.07	C
ATOM	223	C	GLN	B	87	-6.738	-60.618	-33.457	1.00	23.85	C
ATOM	224	O	GLN	B	87	-7.613	-60.012	-34.077	1.00	24.02	O
ATOM	225	CB	GLN	B	87	-7.046	-61.382	-31.097	1.00	24.33	C
ATOM	226	CG	GLN	B	87	-7.873	-62.280	-30.187	1.00	27.24	C
ATOM	227	CD	GLN	B	87	-7.720	-61.943	-28.723	1.00	28.81	C
ATOM	228	OE1	GLN	B	87	-8.567	-62.296	-27.908	1.00	33.25	O
ATOM	229	NE2	GLN	B	87	-6.632	-61.275	-28.375	1.00	29.95	N
ATOM	230	N	ALA	B	88	-5.449	-60.293	-33.521	1.00	23.39	N
ATOM	231	CA	ALA	B	88	-4.996	-59.183	-34.355	1.00	23.78	C
ATOM	232	C	ALA	B	88	-5.257	-59.485	-35.831	1.00	24.73	C
ATOM	233	O	ALA	B	88	-5.655	-58.595	-36.592	1.00	24.72	O
ATOM	234	CB	ALA	B	88	-3.508	-58.909	-34.116	1.00	23.33	C
ATOM	235	N	ARG	B	89	-5.038	-60.735	-36.244	1.00	24.26	N
ATOM	236	CA	ARG	B	89	-5.285	-61.111	-37.636	1.00	24.94	C
ATOM	237	C	ARG	B	89	-6.752	-60.909	-38.013	1.00	25.29	C
ATOM	238	O	ARG	B	89	-7.056	-60.420	-39.104	1.00	24.27	O
ATOM	239	CB	ARG	B	89	-4.904	-62.575	-37.893	1.00	25.14	C
ATOM	240	CG	ARG	B	89	-3.461	-62.774	-38.353	1.00	24.54	C
ATOM	241	CD	ARG	B	89	-3.142	-64.253	-38.510	1.00	25.50	C
ATOM	242	NE	ARG	B	89	-3.809	-64.901	-39.641	1.00	24.93	N
ATOM	243	CZ	ARG	B	89	-3.329	-64.930	-40.882	1.00	25.90	C
ATOM	244	NH1	ARG	B	89	-2.178	-64.336	-41.170	1.00	25.98	N
ATOM	245	NH2	ARG	B	89	-3.979	-65.596	-41.831	1.00	26.36	N
ATOM	246	N	GLY	B	105	5.583	-50.364	-27.741	1.00	23.01	N
ATOM	247	CA	GLY	B	105	4.593	-50.905	-26.827	1.00	23.54	C
ATOM	248	C	GLY	B	105	4.358	-52.380	-27.078	1.00	23.17	C
ATOM	249	O	GLY	B	105	4.449	-52.844	-28.214	1.00	22.69	O
ATOM	250	N	TYR	B	106	4.018	-53.118	-26.026	1.00	22.87	N
ATOM	251	CA	TYR	B	106	3.818	-54.554	-26.159	1.00	22.37	C
ATOM	252	C	TYR	B	106	2.719	-55.018	-27.100	1.00	20.52	C
ATOM	253	O	TYR	B	106	2.867	-56.052	-27.746	1.00	20.50	O
ATOM	254	CB	TYR	B	106	3.632	-55.181	-24.774	1.00	25.08	C
ATOM	255	CG	TYR	B	106	4.864	-55.008	-23.929	1.00	28.19	C
ATOM	256	CD1	TYR	B	106	4.869	-54.153	-22.830	1.00	31.96	C
ATOM	257	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00	31.27	C
ATOM	258	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00	33.13	C
ATOM	259	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00	32.27	C
ATOM	260	CZ	TYR	B	106	7.219	-54.541	-22.487	1.00	33.19	C
ATOM	261	OH	TYR	B	106	8.388	-54.291	-21.802	1.00	35.95	O
ATOM	262	N	VAL	B	107	1.628	-54.270	-27.205	1.00	19.06	N
ATOM	263	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06	C
ATOM	264	C	VAL	B	107	1.015	-54.743	-29.559	1.00	17.45	C
ATOM	265	O	VAL	B	107	0.502	-55.536	-30.346	1.00	16.99	O
ATOM	266	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00	20.95	C

	ATOM	267	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00	21.39	C
	ATOM	268	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00	21.30	C
	ATOM	269	N	SER	B	108	1.991	-53.916	-29.918	1.00	17.96	N
	ATOM	270	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67	C
	ATOM	271	C	SER	B	108	3.197	-55.187	-31.694	1.00	20.38	C
	ATOM	272	O	SER	B	108	3.385	-55.449	-32.884	1.00	21.25	O
	ATOM	273	CB	SER	B	108	3.424	-52.691	-31.508	1.00	19.56	C
	ATOM	274	OG	SER	B	108	4.666	-52.824	-30.837	1.00	19.63	O
	ATOM	275	N	GLY	B	109	3.595	-55.995	-30.710	1.00	19.59	N
	ATOM	276	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03	C
	ATOM	277	C	GLY	B	109	3.311	-58.170	-31.792	1.00	19.61	C
	ATOM	278	O	GLY	B	109	3.579	-58.517	-32.940	1.00	19.24	O
	ATOM	279	N	PRO	B	110	2.206	-58.606	-31.173	1.00	19.20	N
	ATOM	280	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99	C
	ATOM	281	C	PRO	B	110	0.651	-58.761	-33.075	1.00	19.22	C
	ATOM	282	O	PRO	B	110	0.406	-59.371	-34.116	1.00	17.13	O
	ATOM	283	CB	PRO	B	110	0.198	-59.737	-30.778	1.00	20.41	C
	ATOM	284	CG	PRO	B	110	0.998	-59.720	-29.515	1.00	19.81	C
	ATOM	285	CD	PRO	B	110	1.914	-58.528	-29.729	1.00	19.94	C
	ATOM	286	N	GLY	B	111	0.407	-57.462	-32.927	1.00	19.03	N
	ATOM	287	CA	GLY	B	111	-0.160	-56.702	-34.025	1.00	19.60	C
	ATOM	288	C	GLY	B	111	0.764	-56.714	-35.226	1.00	19.59	C
	ATOM	289	O	GLY	B	111	0.330	-56.979	-36.339	1.00	21.10	O
	ATOM	290	N	GLY	B	112	2.043	-56.429	-34.995	1.00	19.78	N
	ATOM	291	CA	GLY	B	112	3.014	-56.417	-36.074	1.00	19.97	C
	ATOM	292	C	GLY	B	112	3.147	-57.783	-36.724	1.00	20.43	C
	ATOM	293	O	GLY	B	112	3.233	-57.896	-37.949	1.00	19.94	O
	ATOM	294	N	LEU	B	113	3.167	-58.828	-35.903	1.00	19.26	N
	ATOM	295	CA	LEU	B	113	3.265	-60.184	-36.429	1.00	19.49	C
	ATOM	296	C	LEU	B	113	2.040	-60.521	-37.274	1.00	18.73	C
	ATOM	297	O	LEU	B	113	2.143	-61.252	-38.255	1.00	18.44	O
	ATOM	298	CB	LEU	B	113	3.405	-61.198	-35.289	1.00	18.38	C
	ATOM	299	CG	LEU	B	113	4.777	-61.270	-34.605	1.00	20.59	C
	ATOM	300	CD1	LEU	B	113	4.656	-62.059	-33.311	1.00	20.01	C
	ATOM	301	CD2	LEU	B	113	5.794	-61.914	-35.538	1.00	20.23	C
	ATOM	302	N	ALA	B	114	0.875	-60.010	-36.892	1.00	18.96	N
	ATOM	303	CA	ALA	B	114	-0.334	-60.292	-37.661	1.00	18.70	C
	ATOM	304	C	ALA	B	114	-0.288	-59.578	-39.019	1.00	19.30	C
	ATOM	305	O	ALA	B	114	-0.602	-60.167	-40.052	1.00	20.62	O
	ATOM	306	CB	ALA	B	114	-1.562	-59.855	-36.889	1.00	16.45	C
	ATOM	307	N	ALA	B	115	0.082	-58.303	-39.000	1.00	20.57	N
	ATOM	308	CA	ALA	B	115	0.167	-57.516	-40.229	1.00	21.84	C
	ATOM	309	C	ALA	B	115	1.140	-58.192	-41.189	1.00	21.58	C
	ATOM	310	O	ALA	B	115	0.815	-58.464	-42.345	1.00	22.14	O
	ATOM	311	CB	ALA	B	115	0.636	-56.108	-39.911	1.00	19.85	C

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ATOM    312  N   TRP B 116       2.334 -58.476 -40.688  1.00 22.12      N
ATOM    313  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22      C
ATOM    314  C   TRP B 116       2.871 -60.434 -42.123  1.00 23.55      C
ATOM    315  O   TRP B 116       3.048 -60.643 -43.329  1.00 22.19      O
ATOM    316  CB  TRP B 116       4.584 -59.367 -40.579  1.00 26.08      C
ATOM    317  CG  TRP B 116       5.699 -60.136 -41.204  1.00 27.40      C
ATOM    318  CD1 TRP B 116       6.473 -59.761 -42.271  1.00 28.30      C
ATOM    319  CD2 TRP B 116       6.168 -61.418 -40.793  1.00 28.77      C
ATOM    320  NE1 TRP B 116       7.401 -60.742 -42.547  1.00 29.04      N
ATOM    321  CE2 TRP B 116       7.234 -61.771 -41.655  1.00 30.37      C
ATOM    322  CE3 TRP B 116       5.794 -62.308 -39.778  1.00 30.49      C
ATOM    323  CZ2 TRP B 116       7.929 -62.981 -41.529  1.00 31.08      C
ATOM    324  CZ3 TRP B 116       6.485 -63.510 -39.653  1.00 31.85      C
ATOM    325  CH2 TRP B 116       7.541 -63.834 -40.527  1.00 32.27      C
ATOM    326  N   SER B 117       2.231 -61.304 -41.338  1.00 21.35      N
ATOM    327  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61      C
ATOM    328  C   SER B 117       0.665 -62.383 -42.940  1.00 23.56      C
ATOM    329  O   SER B 117       0.463 -63.262 -43.780  1.00 23.11      O
ATOM    330  CB  SER B 117       1.167 -63.462 -40.756  1.00 20.72      C
ATOM    331  OG  SER B 117       0.010 -62.889 -40.169  1.00 22.72      O
ATOM    332  N   LEU B 133      11.788 -52.846 -25.860  1.00 23.38      N
ATOM    333  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54      C
ATOM    334  C   LEU B 133      11.209 -54.833 -27.276  1.00 22.84      C
ATOM    335  O   LEU B 133      11.784 -55.619 -28.027  1.00 21.86      O
ATOM    336  CB  LEU B 133      11.328 -54.996 -24.786  1.00 25.48      C
ATOM    337  CG  LEU B 133      11.388 -56.527 -24.780  1.00 27.50      C
ATOM    338  CD1 LEU B 133      12.840 -56.984 -24.866  1.00 28.69      C
ATOM    339  CD2 LEU B 133      10.735 -57.059 -23.509  1.00 28.04      C
ATOM    340  N   THR B 134       9.975 -54.401 -27.499  1.00 21.72      N
ATOM    341  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22      C
ATOM    342  C   THR B 134       9.693 -54.326 -29.986  1.00 20.62      C
ATOM    343  O   THR B 134       9.843 -55.091 -30.932  1.00 20.33      O
ATOM    344  CB  THR B 134       7.716 -54.509 -28.449  1.00 20.99      C
ATOM    345  OG1 THR B 134       7.257 -55.075 -27.210  1.00 20.94      O
ATOM    346  CG2 THR B 134       6.872 -55.073 -29.600  1.00 20.64      C
ATOM   3608  N   LYS B 136      12.595 -53.366 -30.809  1.00 21.46      N
ATOM   3609  CA  LYS B 136      13.886 -53.949 -31.144  1.00 22.79      C
ATOM   3610  CB  LYS B 136      14.713 -54.196 -29.879  1.00 24.70      C
ATOM   3611  CG  LYS B 136      16.183 -54.424 -30.178  1.00 27.75      C
ATOM   3612  CD  LYS B 136      16.998 -54.494 -28.902  1.00 30.17      C
ATOM   3613  CE  LYS B 136      18.479 -54.671 -29.203  1.00 32.33      C
ATOM   3614  NZ  LYS B 136      19.278 -54.641 -27.944  1.00 33.37      N
ATOM   3615  C   LYS B 136      13.793 -55.229 -31.966  1.00 23.46      C
ATOM   3616  O   LYS B 136      14.561 -55.407 -32.912  1.00 23.71      O
ATOM    347  N   TRP B 137      12.868 -56.127 -31.633  1.00 21.78      N
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ATOM    348  CA  TRP B 137      12.753 -57.345 -32.424  1.00 22.06      C
ATOM    349  C   TRP B 137      11.768 -57.202 -33.574  1.00 21.75      C
ATOM    350  O   TRP B 137      11.936 -57.822 -34.623  1.00 21.76      O
ATOM    351  CB  TRP B 137      12.361 -58.552 -31.553  1.00 21.20      C
ATOM    352  CG  TRP B 137      10.990 -58.525 -30.922  1.00 20.23      C
ATOM    353  CD1 TRP B 137      10.696 -58.231 -29.618  1.00 19.62      C
ATOM    354  CD2 TRP B 137       9.748 -58.877 -31.544  1.00 18.68      C
ATOM    355  NE1 TRP B 137       9.349 -58.385 -29.390  1.00 19.31      N
ATOM    356  CE2 TRP B 137       8.743 -58.780 -30.555  1.00 18.97      C
ATOM    357  CE3 TRP B 137       9.383 -59.270 -32.840  1.00 19.75      C
ATOM    358  CZ2 TRP B 137       7.401 -59.058 -30.821  1.00 18.18      C
ATOM    359  CZ3 TRP B 137       8.046 -59.549 -33.107  1.00 18.87      C
ATOM    360  CH2 TRP B 137       7.072 -59.440 -32.099  1.00 18.94      C
ATOM    361  N   LEU B 138      10.741 -56.381 -33.386  1.00 21.61      N
ATOM    362  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15      C
ATOM    363  C   LEU B 138      10.384 -55.558 -35.676  1.00 23.07      C
ATOM    364  O   LEU B 138       9.958 -55.801 -36.809  1.00 22.68      O
ATOM    365  CB  LEU B 138       8.618 -55.305 -33.886  1.00 23.87      C
ATOM    366  CG  LEU B 138       7.312 -55.155 -34.664  1.00 26.48      C
ATOM    367  CD1 LEU B 138       6.672 -56.508 -34.915  1.00 25.34      C
ATOM    368  CD2 LEU B 138       6.383 -54.267 -33.851  1.00 25.90      C
ATOM   3644  N   LYS B 140      12.801 -56.332 -37.241  1.00 27.38      N
ATOM   3645  CA  LYS B 140      13.279 -57.337 -38.182  1.00 28.05      C
ATOM   3646  CB  LYS B 140      13.893 -58.501 -37.401  1.00 29.91      C
ATOM   3647  CG  LYS B 140      15.134 -58.057 -36.635  1.00 31.62      C
ATOM   3648  CD  LYS B 140      15.719 -59.149 -35.757  1.00 33.53      C
ATOM   3649  CE  LYS B 140      16.974 -58.634 -35.055  1.00 34.46      C
ATOM   3650  NZ  LYS B 140      17.692 -59.713 -34.320  1.00 36.17      N
ATOM   3651  C   LYS B 140      12.254 -57.833 -39.212  1.00 27.83      C
ATOM   3652  O   LYS B 140      12.602 -58.562 -40.142  1.00 27.80      O
ATOM    369  N   ILE B 141      10.992 -57.445 -39.052  1.00 26.40      N
ATOM    370  CA  ILE B 141       9.963 -57.818 -40.016  1.00 26.09      C
ATOM    371  C   ILE B 141       9.316 -56.542 -40.530  1.00 25.81      C
ATOM    372  O   ILE B 141       8.353 -56.586 -41.305  1.00 26.10      O
ATOM    373  CB  ILE B 141       8.854 -58.721 -39.405  1.00 26.39      C
ATOM    374  CG1 ILE B 141       8.298 -58.092 -38.127  1.00 26.45      C
ATOM    375  CG2 ILE B 141       9.401 -60.118 -39.145  1.00 28.33      C
ATOM    376  CD1 ILE B 141       7.136 -58.845 -37.549  1.00 26.95      C
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All data sets were collected at 100 K on previously flash frozen crystals. Crystals were equilibrated in a cryoprotectant buffer with 0.1 M NaMES, pH 6.5, 1.44 M $(NH_4)_2SO_4$ 0.4% Triton X-100, and 20% glycerol. Heavy-atom soaks were carried out in the same buffer containing one of the following heavy-atom solutions: 2 mM $HgCl_2$ 1 mM $(NH_4)_2WS_4$, mM $(NH_4)_2OsBr_6$. Crystals were flash-frozen in liquid nitrogen. $HgCl_2$ (form A derivative) and $(NH_4)_2OsBr_6$ derivative data were collected at an R-AXISIIC imaging plate detector mounted on a Rigaku 200HB generator. Native, $HgCl_2$ (form B derivative), and $(NH_4)_2WS_4$ derivative diffraction data were collected at beam-line BioCARS-14B at the Advanced Photon Source, at wavelengths 1.0092 Å, 0.9900 Å and 1.2147 Å respectively. Collection of data on the H_gCl_2, derivative was initially designed for MAD phasing; however, the mercury derivative proved to be unstable to X-rays, and after a two-hour exposure to synchrotron radiation the form A derivative metamorphosed into a different mercury derivative (form B) that was suitable for MIR phasing. All the data were reduced using DENZO and SCALEPACK (Otwinowski & Minor, 1997), and processed with CCP4 programs (CCP4, 1994).

Structure determination and refinement

The structure was solved by multiple isomorphous replacement combined with anomalous scattering of mercuric derivatives (Table 1). Initial MIR phases calculated with program MLPHARE had a mean figure of merit of 0.44 to 2.5 Å, and were improved by solvent flattening and histogram matching using DM. An MIR map was generated which had continuous electron density for most regions of the protein. A model was built with the program O (Jones et al., 1991), and the structure was refined against 1.9 Å data using energy minimization, simulated annealing and B-factor refinement with the program CNS (Brunger et at., 1998). The N-terminal six residues and the C-terminal His-tag had no electron density and were not included in this model. There was no electron density for UDP-GlcNAc.

Conclusion

This first structure of a member of the MurG family of glycosyltransferases lays the groundwork for further mechanistic and structural investigations, which may lead to the design of inhibitors and perhaps even new antibiotics. The work also shows that there can be conserved subdomains even in very different glycosyltransferase families. Information on conserved subdomains will be useful for structure prediction and may help guide experiments directed towards changing substrate specificity.

EXAMPLE 2

This example describes a method of isolating the C-terminal domain of the *E. coli* MurG protein, expressing the domain in *E. coli* cells and utilizing nuclear magnetic resonance (NMR) to determine the ability of compounds to bind.

MurG can also be used to determine the ability of a chemical compound to bind to the C domain by a) determining the start of c domain based on the MurG crystal structure; b) independently expressing the C domain; and c) using NMR methods to identify binding site and/or bound conformation of ligand. The same procedure is used for the acceptor binding domains.

NMR methods are used to identify the protein binding sites nad screen for ligands that bind. The MurG C-terminal domain region of the protein has been expressed independently. The C domain has a much lower molecular weight than the full-length protein. Therefore, the expression of the C domain results in much sharper NMR peaks which will facilitate the NMR interpretation. Also the protin chemical shifts are very sensitive to their environment. Binding of a compound will introduce local environment changes, thus changing the proton chemical shifts. In this way, residues involved in the binding can be differentiated easily from other amino acid residues not involved in binding a ligand. This method has also been used to identify ligands that bind to low molecular weight drug targets (i.e., small proteins).

Relevant references to NMR techniques are: Discovering high-affinity ligands for proteins: SAR by NMR, S. Shuker, P. Hajduk, R. Meadows, and S. Fesik, Science 274, 1531 (1996); Lin Y, Nageswara Rao BD. Structural characterization of adenine nucleotides bound to Escherichia coli adenylate kinase. 1. Adenosineconformations by proton two-dimensional transferred nuclear Overhauser effect spectroscopy. Biochemistry. 2000 Apr 4;39(13):3636-46; and Fejzo J, et al., Chem Biol 1999 Oct;6(10):755-69 (incorporated herein by reference).

The SHAPES strategy is also useful for NMR identification of binding residues, ligands and drug discover which is an NMR-based approach for lead generation in drug discovery. Recently, it has been shown that nuclear magnetic resonance (NMR) may be used to identify ligands that bind to low molecular weight protein drugtargets. Recognizing the utility of NMR as a very sensitive method for detecting binding, we have focused on developing alternative approaches that are applicable to larger molecular weight drug targets and do not require isotopic labeling. A new method for lead generation (SHAPES) uses NMR to detect the binding of a limited but diverse library of small molecules to a potential drug target. The compound scaffolds are derived from shapes most commonly found in known therapeutic agents. NMR detection of low (microM-mM) affinity binding is achieved using either differential line broadening or transferred NOE (nuclear Overhauser effect) NMR techniques. The SHAPES method for lead generation by NMR is useful for identifying potential lead classes of drugs early in a drug design program, and is easily integrated with other discovery tools such as virtual screening, high-throughput screening and combinatorial chemistry.

EXAMPLE 3

This example describes the method of using the three-dimensional structure of *E. coli* MurG to determine the crystal structures of its mutant, enzyme-ligand complex, and MurG homologs, which share the same folding motif. First, a crystalline form of the new protein or the protein complex should be obtained. The E.coli MurG mutants should crystallized in a condition very similar to what we have showed in the method section. The protein-ligand complex can be obtained by soaking the protein crystals in a ligand-containing buffer. Other MurG homologs can be expressed in a His-tagged fashion and purified using affinity colume. Presumably they can be crystallized in a similar way using a detergent as the additive. Next, the diffraction data should be collected and processed. After the data collection, the molecular replacement method is used to determine the unknown structure. Either the whole E. coli MurG protein or one single domain can serve as a search model. This search model can be rotated and translated until the correct orientation is located in the unit cell of this unknown structure. The search model may only represent part of the contents of the asymmetric unit. However, the location of the first model is now already available. While the first location of the search model is fixed, the second round of translation search can be carried out to search more mo, lecules or domains in the asymmetric unit cell. The phases from the final model generated by molecular replacement can be used to calculate

the electron density map. Finally, a model is built based on the electron density map, and the model needs to be refined using program CNS or XPLOR.

EXAMPLE 4

This example describes the method of using the three-dimensional coordinate structure of E. coli MurG to produce a protein fragment that can be used in an NMR-based lead discovery program. The crystal structure reveals the boundaries of the C domain and permits us to design a gene containing only the C domain from the gene containing both domains. The C domain starting at residue 164 and ending at residue 340 was cloned into an expression vector to generate a C-terminal His tag fusion, It was over-expressed in E. coli cells and purified by affinity colume. The protein was shown to be monomeric by size exclusion chromatography and to be soluble at least up to 0.15 mM, a concentration more than adequate for NMR analysis. C domains from other Murg homologues can be similarly expressed and used.

EXAMPLE 5

This example describes the co-crystallization of a MurG protein with a ligand. A MurG-ligand complex is formed by either co-crystallizing MurG protein with appropriate ligand or soaking the MurG crystals in buffers containing appropriate ligand. Co-crystallization is done by pre-mixing the protein sample with a certain amount of substrate or substrate analogs. Then the hanging drop method is used to produce crystals as described infra.

Alternatively, ligans are incorporated into the crystals by soaking the protein crystals in the ligand containing buffer for a period of time to allow for infiltration into the crystal. The time ranges from a couple of hours to a couple of days. The concentration of ligand in the buffer ranges from several milimolar to several hundred mili molar.

DEPOSIT OF COORDINATES

The crystal structure three-dimensional coordinates of the *E. coli* MurG as set forth in Table 1 were deposited with the Protein Data Bank and have been assigned the indicated ID Code (Accession No.) 1FOK.

Although the invention is described in detail with reference to specific embodiments thereof, it will be understood that variations which are functionally equivalent are within the scope of this invention. Indeed, various modifications of the invention in addition to those shown and described herein will become apparent to those skilled in the art from the foregoing description and accompanying drawings. Such modifications are intended to fall within the scope of the appended claims.

Various publications are cited herein, the disclosures of which are incorporated by reference in their entireties.

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